SoK: The Impact of Unlabelled Data in Cyberthreat Detection

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***Abstract*—Machine learning (ML) has become an important paradigm for cyberthreat detection (CTD) in the recent years. A substantial research effort has been invested in the development of specialized algorithms for CTD tasks. From the operational perspective, however, the progress of ML-based CTD is hindered by the difficulty in obtaining the large sets of labelled data to train ML detectors. A potential solution to this problem are semisupervised learning (SsL) methods, which combine small labelled datasets with large amounts of unlabelled data.**

This paper is aimed at systematization of existing work on SsL for CTD and, in particular, on understanding the utility of unlabelled data in such systems. To this end, we analyze the cost of labelling in various CTD tasks and develop a formal cost model for SsL in this context. Building on this foundation, we formalize a set of requirements for evaluation of SsL methods, which elucidates the contribution of unlabelled data. We review the state-of-the-art and observe that no previous work meets such requirements. To address this problem, we propose a framework for assessing the benefits of unlabelled data in SsL. We showcase an application of this framework by performing the first benchmark evaluation that highlights the tradeoffs of 9 existing SsL methods on 9 public datasets. Our findings verify that, in some cases, unlabelled data provides a small, but statistically significant, performance gain. This paper highlights that SsL in CTD has a lot of room for improvement, which should stimulate future research in this field.

***Index Terms*—machine learning, semisupervised learning, cybersecurity, labelling, threat detection**

1. Introduction

Artificial intelligence and especially Machine Learning (ML) are one of the most important drivers of modern IT industry [1]. Specifically, in cybersecurity they can play a crucial role in several tasks, such as vulnerability analysis [2], security intelligence [3], and cyberthreat detection (CTD) [4].

As pointed out by Sommer and Paxson [5], the key to the tremendous success of the so-called *supervised* ML methods is their ability to build models connecting the training input data with the known ground truth information, often referred to as "labels". It is well known, however, that obtaining the ground truth information in cybersecurity is a tough challenge [6]. In computer vision, even a child can say whether a picture shows a cat or a dog. In natural language processing, a linguist – albeit not always a layman – can easily assign linguistic tags to (parts of) the text or assess the quality of its translation. Precise characterization of security events is orders of magnitude more difficult and brings supervised ML methods to a dilemma: they work best when a model is built using an extensive dataset, but the price of labelling such a dataset may be outrageously high. According to Miller et al. [6], an entire company can only afford to label 80 malware samples per day.

On the other hand, unlabelled data is abundant in cybersecurity. Petabytes of network traffic at many levels, monitoring and endpoints logs, as well as many other information sources (e.g., threat intelligence feeds [7]) can be utilized for CTD tasks. Unlabelled data can be used in *unsupervised* ML methods. For instance, clustering proved to be successful for some cybersecurity applications, e.g., analysis of malware families [8]. However, such techniques can only address ancillary tasks, and cannot automate any detection (i.e., classification) mechanism without large amounts of labels that clearly distinguish benign from malicious samples (e.g., [9]).

Semisupervised learning (SsL) [10] has a promise to deliver efficient ML classifiers that require *small* amounts of labelled data by exploiting the information gained from *large* sets of unlabelled data. For instance, in *self learning* (e.g., [11]), labelled data is mixed with unlabelled data to improve performance; similarly, in *active learning* [12] an initial classifier trained on a small labelled dataset can be used to analyze a large set of raw data, and then 'suggest' the most cost-effective samples to label. The SsL setup resembles typical cybersecurity scenarios and, as a result, many works (e.g., [13]–[15]) proposed SsL solutions for diverse CTD tasks.

In a recent study from computer vision, Oliver et al. [16] state, however, that "*the gap in performance between SsL and using only labelled data is smaller than reported*", and that "*a classifier trained on a small labeled dataset with no unlabeled data can reach very good accuracy*". These observations raise the question: is unlabelled data indeed beneficial to SsL and, if so, is it worth the effort? Unlabelled data is cheaper than labelling, but it is not completely 'free'; e.g., its processing and storing costs are not negligible [17], [18].

We researched previous works utilizing the combination of labelled and unlabelled data for CTD and found—surprisingly—that none of such works addressed the *benefits* of unlabelled data in SsL. Identifying such benefits is not simple, because it requires the analysis of the key components that contribute to the development of SsL solutions. Therefore, to the best of our knowledge, it is still unclear whether SsL is advantageous for CTD. This is because prior works adopt evaluation protocols that are not standardized and do not allow to assess whether unlabelled data is cost-effective. Such immaturity serves as the main motivation for our SoK, and our specific goal is to promote

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deployment of SsL methods.

To this end, we formalize a set of requirements derived by a systematic analysis of a realistic deployment of SsL methods in CTD. By following our requirements, it is possible to assess the impact of unlabelled data on the quality of SsL models. Moreover, we propose a novel evaluation framework that can be used to assess existing and future SsL methods in a research environment. Finally, we showcase an application of our framework to perform the first 'benchmark' where we statistically verify the benefits of well-known SsL methods on 9 publicly available datasets for diverse CTD tasks.

Since the scope of this work is well beyond the traditional systematization of previous work, let us outline the **structure** and the **contributions** of this paper.

We begin with the presentation of the background and related research fields in §2. The main focus of this presentation is to illustrate the *challenges of labelling data in CTD*, which is significantly more difficult than in other domains and, hence, motivates the search for solutions that can work with only a small amount of ground truth..

In §3, we formally present the general goal of SsL and analyze its cost structure. The main contributions of this section are an original cost model for SsL in CTD, the definition of the benefit of unlabelled data in SsL, and *the set of requirements* that must be met by research evaluations to ensure that such benefit can be claimed.

In §4, we review the state-of-the-art on SsL for CTD, and analyze to what extent each paper meets the requirements identified in §3. The main conclusion of this analysis is that *no prior work can satisfy all the requirements, and hence demonstrate the benefits of using unlabelled data*. This finding must not be interpreted as a deficiency of prior work; it merely highlights that no one ever questioned the utility of unlabelled data in the deployment of SsL for CTD.

As a first step towards such deployment, we present a new evaluation framework for SsL in §5 and demonstrate its application by assessing 9 well-known SsL methods[1] using 9 datasets in §6. All these contributions provide a constructive approach for assessing the utility of unlabelled data and promote the rollout of SsL solutions for CTD.

Finally, we discuss our findings (§7) and outline the conclusions of our study (§8).

2. Background and Related Work

Obtaining ground truth labels for training ML models is a well-known problem which motivates the investigation of SsL methods (e.g., [19], [20]). However, with respect to other application domains of ML, the process of labelling in CTD is fundamentally harder, making SsL methods particularly attractive here. Let us illustrate all these labelling difficulties which represent the main motivation of our paper.

2.1. Uniqueness of CTD with Respect to Labelling

In some application domains of ML, there exist natural factors that facilitate acquiring labelled data for training ML models. Such factors can be *data sharing* (e.g., [21]), inherent *low cost* of labelling (e.g., the popular CAPTCHAs [22]), or *long-term usage* of labelled data (e.g., ImageNet was collected in 2009 and is still widely used today [23]).

All of these factors are not applicable to cybersecurity due to two intrinsic characteristics. First, the intrinsic confidentiality which strongly discourages data sharing. Second, the constant adaptation of attackers as well as the growth and the evolution of the environments being protected lead to the phenomenon known as *concept drift* [24], i.e., a fundamental change (gradual or abrupt) of the respective data generation processes. This latter issue is crucial, as it conflicts with the underlying 'iid' assumption[2] of ML and hence adversely affects its reliability in production environments [5].

The peculiarities of CTD are especially clear in comparison to computer vision. In image recognition problems, the underlying ground truth is clear and stable. "A cat will always be a cat, whereas a dog will always be a dog" [25], and a person can usually distinguish between two image classes very well [26], although specific applications may demand more informed opinions (e.g., physicians for cancer diagnoses [27]). Moreover, after acquiring such labelled data, it is possible to apply *data augmentation* [28] strategies to increase its effectiveness. For instance, adding some noisy pixels or mirroring the image allows one to create a new image that is different from the original but still has the same ground truth.

In contrast, all of the following situations can occur in CTD:

- a malicious sample is benign elsewhere [5];
- a malicious sample can be purposedly crafted to represent a benign sample [29];
- a benign sample today becomes a malicious sample tomorrow (the so-called 'label shift' [30]).

To aggravate the problem, verifying the ground truth of a sample is hard even for security experts, requiring further verifications [31]. Finally, data augmentation is difficult to apply in CTD: for instance, changing a *single* byte can turn many malicious samples into benign samples [32].

Without loss of generality, we can state that a dataset that is usable for realistic CTD applications of ML must meet the following criteria [33]–[35]:

- It must be *large* enough to capture all the underlying characteristics of the environment to protect, and of the threats to defend against [5].
- The ratio of benign/malicious samples must be *balanced* enough to allow efficient detection without generating excessive false alarms [36].
- It must have *accurate ground truth* [31].
- It must be *continuously updated* [24].

All these peculiarities make obtaining adequate labelled datasets for CTD a tougher challenge than in other domains.

2.2. Specific Labelling Issues in CTD

We analyze the common procedures, and corresponding issues, to obtain labelled data for CTD, split in three

1. Benchmarking *all* SsL methods used in prior works is clearly unfeasible.

2. iid=independent and identically distributed random variables.

broad areas: Network Intrusion Detection (NID), Phishing Website Detection (PWD), Malware Detection (MD) [4], [37].

Network Intrusion Detection. The detection of intrusions within a network perimeter can greatly benefit from ML [4], [38] when labelled datasets are available. In the case of NID, such datasets contain samples providing network-related data. Well-known formats include full Packet Captures (PCAP) or Network Flows (NetFlows) [39]. PCAP provides low-level information but it is not usable if the traffic is encrypted[3]; moreover, storing and analyzing PCAP is computationally expensive. In contrast, the NetFlow format mitigates these issues by providing a high-level overview of network communications between two endpoints while still enabling an appreciable detection performance [39], [40]. Other common data formats are DNS records for investigation of malicious domains [41], and SNMP for monitoring of specific hosts [42]. Regardless of the data-type, a common problem in NID is that every network is unique [5], [36]. An anomalous behavior in one network may be normal in another network, hence preventing a reliable 'transfer' of ML models. Moreover, obtaining accurate ground truth is tough for both *benign* and *malicious* samples. Most existing NID datasets used in research are created by infecting some machines in a controlled network environment with known malware, and capturing the traffic of the simulated network (e.g., [43]–[45]). Such approach is difficult to apply in reality. Verifying that a sample is truly legitimate requires ensuring that both hosts (the source and destination) 'connected' by the specific traffic sample are not malicious. If one of these hosts is compromised via an unknown vulnerability then labelling all the traffic generated by such host as benign can lead to poisoning attacks [29]. Acquiring *malicious* samples is also difficult, because it requires compromising *real* machines with malware, hence exposing the network to external threats. Another problem is to consider all traffic originating from an infected machine is malicious, as some of its data may be generated by legitimate network activities (e.g., ARP messages). All such challenges increase the difficulty of obtaining representative datasets for NID [46].

Phishing Website Detection. Phishing attacks can be launched in various ways, e.g., via email or social networks [47]. In this paper, we focus on the detection of phishing websites because phishing usually involves luring the victim to enter some information on a (phishing) website. Attackers can easily create 'squatting' websites that are difficult to detect [48], making them a rampant threat [49]. Datasets for PWD may include diverse data derived from, e.g., the URL (its length or the usage of some characters), the DNS record (a recent website is more likely to be a phishing hook), the HTML code (phishing websites have many pointers to external domains), and even the image of the landing page (most phishing hooks are similar to legitimate websites) [50]–[53], each having its pros and cons [54]. The most common way to create labelled datasets for PWD is to use public lists of benign or malicious pages (e.g., AlexaTop or PhishTank). The webpage can be visited and the relevant information extracted to compose a given dataset [55]. In general, this process makes labelling for PWD easier than in NID, because verification is simple through expert knowledge [56]. Moreover, the ground truth of a website is independent on the target system (phishing page will 'always' be malicious), enabling model transfer. However, such advantage presents some risks. For instance, the PWD embedded in the Google's Chrome web-browser was reverse engineered, allowing to craft phishing webpages that bypass detection [57]. Therefore, model transfer without an influx of new labelled data makes a PWD unreliable.

Malware Detection. The advent of data-driven solutions, such as ML, allowed the identification of malware variants which bypass traditional rule-based systems [9]. Even commercial products leverage ML [58], which can be used for both static or dynamic MD [59], [60]. The complexity of generating labelled datasets for MD falls between PWD and NID. Obtaining a large corpus of files (benign or malicious) for MD is not difficult per-se, as it can be done via public repositories. However, relying on such data without verifying the ground truth is risky. For instance, well-known marketplaces were recently found to contain malicious applications [61]. Treating such applications as *benign* exposes to *poisoning* attacks, and hence further verifications are required. Such verifications are, however, challenging: some web-services can automatically analyze an input (e.g., VirusTotal), but such services can disagree [37], leading to unreliable results that require costly validation by experts [62]. A possible workaround is using 'collective wisdom' techniques that aggregate the results from diverse antimalware engines [63]; recent works also propose to sanitize 'noisy' labels in the training data [64].

Takeaway: Acquiring labelled data for CTD is challenging. To facilitate the development of ML-solutions, it is necessary to investigate approaches that can work when most of the data is not provided with the ground truth, such as SsL methods.

2.3. Focus of the Paper

Combining labelled and unlabelled data to improve the proficiency of ML methods can be done in many ways. This SoK paper focuses on development of ML-systems for CTD, devised by using (i) *small* sets of labelled data (ii) together with *large* sets of unlabelelled data. Such settings align with the definition of 'Semisupervised Learning' by Oliver et al. [16]. To clarify our focus, we describe two exemplary techniques, illustrated in Fig. 1: *self learning via pseudo-labelling* (e.g., [65]) and *active learning via uncertainty-sampling* (e.g., [66]), both associated with SsL [67]–[69].

In *self learning*, the task of a ML model is to automatically learn from itself. In the specific case of *pseudo labelling*, the intuition is to first train a ML model on a (small) set of labelled data ($\mathbb{L}$ in Fig. 1), and then use such model to predict the label of a (large) set of unlabelled data ($\mathbb{U}$ in Fig. 1). Such 'pseudo-labels' are then used to retrain the model on a mixed dataset, containing both the correct labels of $\mathbb{L}$ and the pseudo-labels of $\mathbb{U}$. To avoid

3. Encrypted payloads also make labelling activities more difficult due to the impossibility of verifying the ground truth of a network packet.

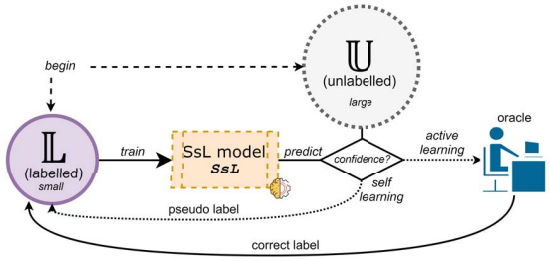

Figure 1: Active Learning and Pseudo Labelling.

using potentially wrong labelled data, the retraining can be done by using only the pseudo-labelled samples with a high *confidence* estimated by the model.

In *active learning*, the ML model interacts with an oracle (realistically, with a human) to improve its learning phase. In the specific case of *uncertainty sampling*, the idea is to first train a ML model on a (small) set of labelled data, $\mathbb{L}$, and then use such model to analyze a (large) set of unlabelled data, $\mathbb{U}$. The analysis is focused on 'suggesting' to the oracle which samples in $\mathbb{U}$ should be correctly labelled to improve the performance, and the suggestion is based on the *confidence* of the model on the samples in $\mathbb{U}$. Intuitively, the model can learn 'more' from samples with a low confidence [70]. The oracle then assigns the correct ground truth to such samples, which are inserted into $\mathbb{L}$ and used to retrain the model—using a correctly labelled dataset.

2.4. Related Work

There exist many learning paradigms that focus on providing reliable models under the assumptions of scarce label availability; often, the term 'Semisupervised Learning' is used to describe techniques that deviate from our definition. We summarize a few orthogonal areas to our work.

Federated learning [71] aims to develop a 'collective' ML-model by combining 'small' ML-models trained on small datasets. Despite some risks (e.g., poisoning [72]) recent efforts applied it successfully even in privacy-sensitive settings [73]. However, federated learning makes no usage of unlabelled data, and the final labelled dataset is huge.

Few-shot learning has the goal of identifying unknown classes when only very few (or even zero [74]) labels are available. For example, by finding the most relevant parameters of a baseline feature extractor, it is possible to generalize on unseen classes [75]. These approaches—conceptually similar to 'anomaly detection'—are thus tailored for detecting novel attacks, and showed promising achievements even in CTD (e.g., [76]). However, they assume a large amount of initial labelled samples for the 'known' classes. As an example, the authors of [77] train their one-class classifiers on 80% of the available samples for the 'normal' class. Similarly, the ML-NIDS in [74] can detect 14 'unseen' attacks, but is trained on over 200k samples spanning over 12 'known' classes.

Representation learning focuses on finding the features that maximize the performance of a ML classifier [78]. It is possible to use unlabelled data to fine-tune such selection (e.g., [79]–[83]). Such procedures are ancillary to detection tasks, and hence outside our scope. As an example, the anomaly detector in [78] mixes a large set of unlabelled data with a small set of labels to identify the most representative features: however, once such features are identified, the experiments for the actual 'detection' are performed by using 60% of the (fully labelled) available data to train the classifier.

Finally, *lifelong learning* aims to update ML models over-time [84], [85], which can be done by exploiting future (unlabelled) data streams; an assumption shared by active learning. However, sometimes the initial cost of labelling is neglected (this is the same problem as few-shot learning). An exemplary case is Tesseract [86], focusing on time-aware MD. The idea of Tesseract is using, among others, active learning strategies to improve over time: despite increasing performance by 20% with 700 additional labels, the initial deployment of Tesseract requires huge amounts of correct labels (i.e., more than 50K). Hence, some applications of active learning may have assumptions that deviate from ours.

We stress that our paper focuses on CTD. As such, any proposal that uses SsL for a different security-related task (e.g., fingerprinting [87]) is orthogonal to this paper.

3. Semisupervised Learning for CTD

In contrast to obtaining ground truth information, acquiring unlabelled data for CTD is relatively straightforward.

Semisupervised Learning (SsL) aims to combine unlabelled with labelled data to devise ML models, which leads to the following question: "what is the *benefit* of unlabelled data?". Only by answering this question it is possible to understand the role that SsL can play in CTD.

Let us begin our research by introducing SsL and its relationship with traditional supervised learning (SL) methods.

3.1. Introduction to Semisupervised Learning

Any ML model requires to *learn* from data so that, after its deployment, it provides insightful analyses on *future* and unseen data, which we denote as $\mathbb{F}$. For those ML methods that require supervision (such as SL and SsL), the learning is done by means of *labelled* data. To achieve the best performance, supervised models should be trained on a huge and fully labelled dataset, $\bar{\mathbb{L}}$. Creating such $\bar{\mathbb{L}}$ may, however, be prohibitive. In contrast, under the constraint of a limited labelling budget, $\mathcal{L}$, the amount of labelled data will be smaller, $\mathbb{L}$, and the resulting model may be inferior to the model that could have been built using $\bar{\mathbb{L}}$.

SsL aims at bridging the gap between labelling effort and the model quality, by using $\mathcal{L}$ alongside a large *unlabelled* dataset, $\mathbb{U}$, which is cheap to acquire. The resulting model should attain a better performance on $\mathbb{F}$ than a model built with same $\mathcal{L}$ but without using $\mathbb{U}$.

For instance, consider the two methods described in §2.3. In self-learning, the model should achieve a better performance after retraining on the 'pseudo-labels' from $\mathbb{U}$ than the initial learner. In active learning, the model trained on the $\mathbb{L}$ with the 'suggested' samples from $\mathbb{U}$ should outperform a model trained on a $\mathbb{L}$ derived from

the same labelling budget $\mathcal{L}$, but without any 'suggestions' derived by $\mathbb{U}$.

We now formally define the abovementioned scenarios. Without loss of generality, any CTD task can be seen as 1+N *classification* ML problem, where samples are either benign, or belong to one among N malicious classes. For simplicity, in the remainder we will consider the *binary*-classification setting; all our considerations have a straightforward extension to the multi-classification setting.

Let $\mathcal{L}$ be a given labelling *budget*. Let $\mathbb{L}$ be any *labelled* dataset containing sample-label pairs, obtained by using $\mathcal{L}$. The composition of any labelled dataset is determined by its *size*, $|\cdot|$, and its *class balance ratio*, $\rho(\cdot)$, which is a 1+N dimensional vector defining the distribution of its samples in percentages. Let $|\mathbb{L}|$ and $\rho(\mathbb{L})$ denote the size and class balance ratio[4] of $\mathbb{L}$. Let $\overline{\mathbb{L}}$, with $\rho(\overline{\mathbb{L}})$, be a superset of $\mathbb{L}$.

Let $\mathbb{U}$ be an *unlabelled* dataset containing samples of which the ground truth is not known, with $|\mathbb{L}| \ll |\mathbb{U}|$.

Finally, let $\mathbb{F}$ be another labelled dataset whose $|\mathbb{F}|$ and $\rho(\mathbb{F})$ should enable meaningful performance assessments. Because $\mathbb{F}$ represents future data, $\mathbb{F} \cap (\overline{\mathbb{L}} \cup \mathbb{U}) = \varnothing$. Let μ be any performance *metric*, e.g., accuracy or F1-score.

An illustration of the upcoming definitions is in Fig. 2.

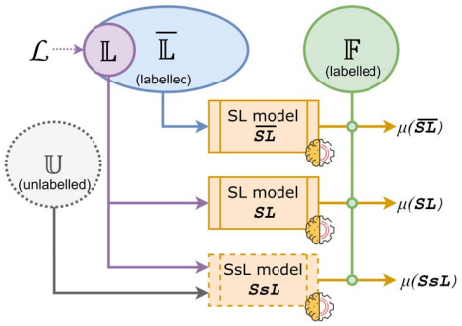

Figure 2: Semisupervised Learning w.r.t. Supervised Learning.

A Supervised Learning (SL) method uses a labelled dataset to train a model that, after deployment, can predict the ground truth of unseen samples (i.e., in $\mathbb{F}$) obtaining a certain performance $\mu(\cdot)$. To achieve optimal performance, the dataset used to train a model via SL should be comprehensive, that is, it should be adequately *large* and *balanced*. As a direct consequence, a model trained on a very small dataset will have a subpar performance. Let $\overline{SL}$ be a model trained on $\overline{\mathbb{L}}$, and SL be a model trained on $\mathbb{L}$: if $|\mathbb{L}| \ll |\overline{\mathbb{L}}|$ then $\mu(SL) < \mu(\overline{SL})$, irrespective of $\rho(\mathbb{L})$. In the remainder, we assume[5] that training $\overline{SL}$ on $\overline{\mathbb{L}}$ results in optimal $\mu(\overline{SL})$, and that $|\mathbb{L}| \ll |\overline{\mathbb{L}}|$.

We can now provide the following definition:

Definition 1. The *goal* of a Semisupervised Learning (SsL) method is using $\mathbb{U}$ alongside any $\mathbb{L}$ obtained with $\mathcal{L}$ to devise a model SsL. After deployment, such SsL should predict the ground truth of the samples in $\mathbb{F}$ by achieving a performance $\mu(SsL)$ that is: $\mu(SL) < \mu(SsL) \leq \mu(\overline{SL})$.

4. If N=1, an example is: $\rho(\mathbb{L}) = (60,40)$, i.e., 60% of samples in $\mathbb{L}$ are benign, and 40% are malicious.

5. Finding the exact size and balance of a dataset that yield the best performance is a NP-hard problem.

From Def. 1, we derive that assessing the *benefits* of SsL methods is linked with SL, because only by comparing[6] SsL with SL (and $\overline{SL}$) it is possible to determine the role of $\mathbb{U}$.

3.2. Cost model of SsL for CTD

Let us interpret the abstract descriptions in §3.1 from the perspective of a real organization interested in deploying a SsL solution for CTD. An illustration is provided in Fig. 3.

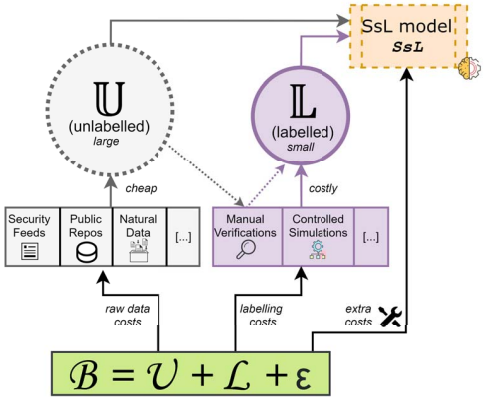

Figure 3: Proposed cost model for deployment of SsL methods.

In the real world, a resource *investment* is required for integrating any new solution, and the decision to deploy such solution depends on its estimated return on investment (ROI). Assessing such ROI demands the definition of a *cost model* that allows practical comparisons to support decisions [88].

Huge amounts of data, $\mathbb{U}$, can be easily obtainable. An organization can have a rough idea about the nature of such data, but the impossibility of determining the ground truth without costly manual inspection makes it necessary to treat all its samples as unlabelled.

However, any SsL model necessitates at least a small amount of labelled data, $\mathbb{L}$. Such $\mathbb{L}$ can be acquired either before and independently from $\mathbb{U}$, or by using $\mathbb{U}$. For instance, $\mathbb{L}$ can be obtained by verifying uncertain labels, manually labelling existing data, or even by creating new labelled data via controlled simulations (§2). In addition, like all ML-solutions, SsL models must undergo ancillary operations (e.g., feature engineering, data cleaning, and training [4]).

We can hence define the *cost model* for development of SsL solutions[7]. Deployment of a semisupervised model SsL requires to invest some *budget*, $\mathcal{B}$. Such budget can be seen as the contribution of three components $\mathcal{U}$, $\mathcal{L}$ and ε. Specifically:

- $\mathcal{U}$ represents the investment for obtaining (and, if necessary, maintaining) the unlabelled data $\mathbb{U}$;
- $\mathcal{L}$ is the investment for generating $\mathbb{L}$. Specifically, $\mathcal{L}$ is used to ensure that any sample $x \in \mathbb{L}$ has the

6. Doing this, however, requires that $\mathbb{L}$ is a strict subset of $\overline{\mathbb{L}}$: otherwise (i.e., if $\mathbb{L} \cup \overline{\mathbb{L}} \neq \overline{\mathbb{L}}$) it would not be fair to compare $\mu(SL)$ with $\mu(\overline{SL})$ and, consequently, with $\mu(SsL)$. This is because the performance difference may be due to the samples in $\mathbb{L}$ not included in $\overline{\mathbb{L}}$.

7. TtBooK, we are the first to propose a cost model that is specific for SsL.

correct label. Such $\mathcal{L}$ can be used all at once or at different times: for instance, it is possible to reserve a portion for subsequent labelling rounds that depend on $\mathbb{U}$ (e.g., active learning).

- $\varepsilon(SsL)$ is used for any *extra* operation for developing the model SsL that is not related to labelling the samples in $\mathbb{L}$. For instance, it can be used to (i) conduct preliminary analyses on $\mathbb{U}$, (ii) tune SsL, (iii) process data, as well as for any (iv) computational costs.

By using $\mathcal{L}$, the organization eventually obtains a labelled dataset $\mathbb{L}$, whose composition (i.e., $\rho(\mathbb{L})$ and $|\mathbb{L}|$) depends on the cost of labelling each individual sample x in $\mathbb{L}$; let $\mathcal{C}_x$ denote such *cost*. We can express our cost model by formally defining $\mathcal{B}(SsL)$ with the following Equation:

$$\mathcal{B}(SsL) = \mathcal{U} + \mathcal{L} + \varepsilon(SsL), \text{ where } \mathcal{L} = \sum_{x \in \mathbb{L}} \mathcal{C}_x \quad \text{(Eq. 1)}$$

Such budget $\mathcal{B}$ represents an *investment* whose *return* is based on the performance achieved by SsL after deployment, that is, $\mu(SsL)$. The ROI of any solution can be expressed as the ratio between its expected performance and its development budget [89]; in the case of SsL: $\text{ROI}(SsL) = \mu(SsL)/\mathcal{B}(SsL)$.

We note, however, that $\mu(SsL)$ depends on 'future' data which is, by definition, *not* available to the organization. It is hence necessary to conduct thorough experimental evaluations *in advance* which can certify that: (i) a given SsL (or its generative SsL method) will yield appreciable $\mu(SsL)$ when deployed in practice; and that (ii) allow comparisons of similar techniques by assessing their costs and benefits. If such evaluations are conducted on a dataset with a similar distribution of 'future' data, then the resulting $\mu(SsL)$ will approximate the real deployment performance. In this case, it is possible to estimate the potential ROI of a SsL solution and facilitate informed decisions for their deployment. Nevertheless, after deployment, real organizations must regularly perform new evaluations to mitigate the likely concept drift (cf. §2.1).

Takeaway: by investing $\mathcal{B}$, an organization can cheaply obtain $\mathbb{U}$ and compose a small $\mathbb{L}$ which are used to develop a model SsL. Such model will only be developed (and deployed) if its estimated ROI is more beneficial than other solutions, i.e., if evaluations conducted *in advance* show that SsL outperforms solutions that require a lower or similar budget.

3.3. Requirements for Evaluation of SsL Methods

Let us explain how to conduct evaluations that allow to estimate the ROI and, hence, gauge the benefits of SsL.

In research, evaluations of ML are done by means of fully labelled datasets, which should represent realistic scenarios and hence must be unbiased. Let $\mathbb{D}$ be one of such datasets[8]. From Def. 1, a SsL model aims at $\mu(SL) < \mu(SsL) \leq \mu(\overline{SL})$. Therefore, the source dataset $\mathbb{D}$ must be used to to derive the four sets $\mathbb{F}$, $\mathbb{U}$, $\mathbb{L}$, and $\bar{\mathbb{L}}$ necessary to compute such performance. To align the evaluation with real deployment use-cases, the creation of these sets must be done by taking $\mathcal{B}$ and, hence, $\mathcal{L}$ into account. Note that $\mathbb{F}$ is only used to assess the performance on simulated 'unknown' data, which is not available in advance. Therefore, using $\mathbb{F}$ to 'cherry pick' the samples to put in $\mathbb{L}$ is prohibited [90].

We can now define the 7 requirements, applicable to any CTD task, that must be upheld to ensure unambiguous assessment of the *benefits* of SsL methods.

Req. 1 (Lower Bound)**.** It is necessary to evaluate a lower bound model that only uses $\mathcal{L}$ and makes no use of $\mathbb{U}$. In other words, train a model SL on $\mathbb{L}$ and evaluate its performance on $\mathbb{F}$ as $\mu(SL)$. To avoid bias[9], such $\mathbb{L}$ must be chosen by *random* sampling from $\mathbb{D}$ subject to $\mathcal{L}$. **Motivation:** The SL represents the true baseline[10], allowing to assess the benefit (and, hence, compare the ROI) of any model SsL that uses $\mathbb{L}+\mathbb{U}$. For instance, if $\mu(SsL) \approx \mu(SL)$ then there is no practical benefit in using the unlabelled data in $\mathbb{U}$; it may also be that $\mu(SsL) < \mu(SL)$, meaning that using $\mathbb{U}$ is detrimental.

Req. 2 (Ablation Study)**.** It is necessary to always consider a 'vanilla' model $\underline{SsL}$ that uses $\mathbb{U}$ in a trivial way together with an $\mathbb{L}$ randomly sampled from $\mathbb{D}$. The aim is minimizing the degree of supervision[11] involved by using $\mathbb{U}$. **Motivation:** The 'vanilla' $\underline{SsL}$ allows to gauge (i) the smallest improvement provided by $\mathbb{U}$ via comparisons with SL; and also (ii) the smallest *cost* induced by using $\mathbb{U}$, because the randomness of $\mathbb{L}$ and the lack of supervision makes the corresponding ε minimal. Moreover, $\underline{SsL}$ serves as a baseline for an *ablation study* [20], to simulate worst case scenarios in which any operation that relies on $\mathbb{U}$ to refinely compose $\mathbb{L}$ is not functional in practice.

Req. 3 (Upper Bound)**.** It is necessary to train an upper bound model $\overline{SL}$ on $\bar{\mathbb{L}}$ and evaluate its performance on $\mathbb{F}$ as $\mu(\overline{SL})$. **Motivation:** The $\overline{SL}$ serves to assess the performance achievable by augmenting $\mathbb{L}$ until it reaches $\bar{\mathbb{L}}$. Moreover, if $\mu(SL) \approx \mu(\overline{SL})$, then investing in $\mathcal{U}$ to develop any SsL method may not be worth it in the first place.

Req. 4 (Statistical Significance)**.** It is necessary to verify the statistical significance of any evaluation result. **Motivation:** Evaluations of SsL involve a lot of randomness and uncertainties. The huge search space for composing $\mathbb{L}$ from $\mathbb{D}$ may lead to erratic results: in some cases $\mu(SsL) > \mu(SL)$, but the opposite can also be true. Moreover, sometimes $\mu(SsL) \approx \mu(SL)$ meaning that further tests are required to determine if SsL is superior to SL. Hence, different draws of $\mathbb{L}$ (and, preferably, also of $\bar{\mathbb{L}}$ and $\mathbb{F}$) must be assessed and conclusions must be drawn after statistically significant comparisons[12].

8. $\mathbb{D}$ can be subject to some preliminary preprocessing.

9. Labelling is not deterministic, and in realistic scenarios it is not possible to know *in advance* the effectiveness of labelling.

10. Such SL should aim at maximizing the gain from $\mathbb{L}$ (and hence $\mathcal{L}$), but it should not be overtuned (leading to overfitting and astronomical ε), nor it should be 'sabotaged' with incorrect configurations to inflate results.

11. Depending on the context, there can be many ways of devising $\underline{SsL}$. As an example, in pseudo-labelling, a 'trivial' way is using all pseudo-labels regardless of their confidence; whereas, in active learning, a 'trivial' way is labelling randomly chosen samples (instead of those with least confidence).

12. Note that such efforts go beyond traditional 'cross-validations' [86].

Req. 5 (Transparency)**.** It is necessary to ensure full transparency on the composition of $\mathbb{L}$, $\overline{\mathbb{L}}$, $\mathbb{U}$ and $\mathbb{F}$. This implies: specifying *size* of each dataset (both in absolute numbers, and with respect to $\mathbb{D}$); and the *balance ratios* in terms of class composition. **Motivation:** Claiming that a given SsL method is effective when using only "1% of the data" is not as enticing if $\mathbb{D}$ has 1M samples. Moreover, the balance ratio can significantly alter the results when small datasets are considered (as we will show in our evaluation). This requirement also serves to estimate $\mathcal{L}$ and $\mathcal{U}$.

Req. 6 (Reproducibility)**.** Any evaluation must be supported with information that allow its reproducibility [91], [92]. **Motivation:** aside from obvious reasons, it serves to approximate ε.

Req. 7 (Multiple Settings)**.** It is necessary to evaluate any model by considering multiple deployment settings, e.g., diverse datasets. **Motivation:** for practical deployments, the samples in $\mathbb{D}$ must resemble the true distribution at inference, and CTD scenarios can vary (cf. §2).

The intuition behind our requirements is that any model SsL developed with a given SsL method must be compared against the three baselines of Regs. 1–3. By doing so, it is possible to measure the added value of SsL, building on $\mathbb{U}$, potentially creating a better $\mathbb{L}$, but with a specific extra cost ε. It is implicit that any model-to-model comparison must be done under the assumptions of identical $\mathcal{L}$.

We now provide our formal definition of the utility of $\mathbb{U}$.

Definition 2. Unlabelled data $\mathbb{U}$ used to develop the model SsL is *beneficial* if it can be shown that: (i) $\mu(SL) \ll \mu(\overline{SL})$, and (ii) ROI($SsL$) is better than both ROI(SL) and ROI($\underline{SsL}$).

Since SL does not use $\mathcal{U}$, and $\underline{SsL}$ should minimize ε (w.r.t. SsL), it follows that $\mu(SsL)$ must be greater than $\mu(SL)$ and also greater or equal than $\mu(\underline{SsL})$. To justify deployment of a new SsL method, its evaluation must show that Def. 2 holds in different settings.

Takeaway: Research evaluations of SsL methods require to train and test (i) multiple models (ii) many times and in (iii) different scenarios, while disclosing full information of the experimental settings. If these requirements are met, it is possible to assess the deployment benefits of a SsL method.

4. State-of-the-Art

We analyze the state-of-the-art w.r.t. the proposed requirements (§3.3), and provide a summary in Table 1. Let us describe our methodology, and then discuss the main findings.

4.1. Methodology

To assess the extent to which existing works meet the proposed requirements, we perform a systematic literature survey. Such process is organized in three phases: *search*, *screening*, *investigation*. To reduce bias, all phases involved two researchers who worked *independently*, and whose individual findings were discussed in weekly meetings.

4.1.1. Search. The first phase focused on finding all literature linking (even remotely) SsL with CTD. To this purpose, we systematically searched well-known scientific repositories. Such repositories include IEEE Xplore, Google Scholar, and ACM Digital Library; but we also extended our search to the proceedings of the top security conferences. In particular, we searched for the following keywords:

$$(semi\text{-}supervised \vee semisupervised \vee semi\ supervised \vee active) \wedge (network \vee malware \vee phishing \vee intrusion)$$

which had to be included either in the title or in the abstract. Any work that was not peer-reviewed was excluded, and we looked for papers published after 2007. The results of such search formed an initial corpus of papers, which was further extended with all papers that either cited, or were cited by, a given work (and that included same or similar keywords); as well as with papers that the authors autonomously found during their daily duties (e.g., reviewing).

4.1.2. Screening. After obtaining the corpus of candidate papers, we studied them with the intent of determining which papers fall within our scope. By referring to §2.3, a paper had to meet three criteria: (i) focus on CTD, (ii) using unlabeled data, (iii) in combination with *small* sets of labelled data[13]. After several discussions between the two researchers, this phase resulted in the set of 48 papers reported in Table 1. To the best of our knowledge, Table 1 represents the current state-of-the-art of SsL for CTD.

4.1.3. Investigation. Those papers that met all the inclusion criteria were then further analyzed, with the goal of assessing their compliance with the proposed set of requirements. The results are in Table 1, which is organized as follows. We distinguish the papers on the basis of the three main CTD areas of interest (NID, PWD, MD); cells with a gray background denote papers that specifically consider 'active learning' approaches. For each paper we compare it with our requirements: a ✓ (resp. ✗) denotes that a requirement is met (or not).

- For Req. 1, we use ◐ if it is not explicitly mentioned that $\mathbb{L}$ was randomly drawn, and ✗ when either the SL is missing, or when such SL uses a different $\mathcal{L}$.
- For Req. 2, we use ✓ if the paper considers a SsL model that is completely unbiased and can serve as an ablation study; ◐ if the SsL models are trained on a unbiased random $\mathbb{L}$, but cannot serve as an ablation study due to 'overuse' of $\mathbb{U}$; and ✗ if the provided information is insufficient to determine the absence of bias in $\mathbb{L}$.
- Req. 3 is binary, but we also consider as ✓ when the SsL method is trained on a very large set of correct labels.

13. The term 'Semisupervised Learning' has been used in many ways (§2.4).

TABLE 1: State-of-the-Art of SsL for CTD w.r.t. our evaluation requirements. A '*' indicates a resource not available as of Sept 2021. Gray cells denote active learning. **All these works had a different scope than our paper, hence not meeting our requirements does not invalidate their contribution.**

Task	Paper (1st Author)	Year	Lower Bound	Ablation Study	Upper Bound	Stat. Sign.	Transparency		Repr.	Dataset
							Labels	*Balance*		
Network Intrusion Detection	Li [93]	2007	✓	✓	✗	✗	✓	✓	◐	NSL-KDD
	Long [94]	2008	✓	✓	✗	◐	✓	✗	◐	NSL-KDD
	Görnitz [95]	2009	✓	✓	✗	◐	✓	✓	✗	Private
	Seliya [96]	2010	✓	✓	✗	✗	✓	✓	◐	NSL-KDD
	Symons [97]	2012	✗	✓	✓	◐	✓	✗	✗	Kyoto2006
	Wagh [98]	2014	✗	✗	✗	✗	✓	✓	◐	NSL-KDD
	Noorbehbahani [35]	2015	✗	◐	✓	✗	✓	✓	◐	NSL-KDD, Custom
	Ashfaq [99]	2017	✗	◐	✗	✗	✓	✗	◐	NSL-KDD
	Qiu [67]	2017	✗	◐	✓	✗	✓	✓	✗	Custom
	McElwee [100]	2017	✗	◐	✓	✗	✓	✗	◐	NSL-KDD
	Kumari [68]	2017	✓	◐	✗	✗	✓	✗	◐	NSL-KDD
	Yang [101]	2018	◐	✓	✓	✗	✓	✗	✗	NSL-KDD, AWID
	Gao [102]	2018	✓	◐	✗	✗	✓	✗	✗	NSL-KDD
	Shi [103]	2018	◐	◐	✗	✗	✓	✗	✗	NSL-KDD
	Yao [36]	2019	◐	◐	✓	✗	✓	✓	◐	NSL-KDD
	Yuan [104]	2019	✗	◐	✗	◐	✓	✓	◐	NSL-KDD
	Zhang [65]	2020	◐	✗	✓	◐	✓	✗	◐	NSL-KDD
	Hara [105]	2020	✗	◐	✓	✗	✗	✗	✗	NSL-KDD
	Ravi [106]	2020	✓	✗	✗	✗	✓	✗	✗	NSL-KDD
	Gao [107]	2020	✗	✓	✓	✓	✓	✓	✗	NSL-KDD
	Li [108]	2020	✗	◐	✓	✓	✓	✗	◐	NSL-KDD, Private
	Zhang [70]	2021	◐	◐	✗	◐	✗	✓	◐	CICIDS2017, CTU13
	Liang [109]	2021	✓	◐	✓	◐	✓	✓	◐	NSL-KDD
Phishing Detection	Gyawali [110]	2011	✗	✓	✓	✗	✓	✓	◐	Private
	Zhao [111]	2013	✓	✓	✓	✓	✗	✓	✓*	DetMalURL
	Gabriel [15]	2017	◐	◐	✗	✗	✗	✗	◐	Private
	Yang [112]	2017	✓	◐	✗	✗	✓	✓	◐	Private
	Bhattacharjee [113]	2017	✗	✓	✗	◐	✗	✗	◐	Private
	Li [55]	2017	✓	✓	✓	◐	✓	✓	✗	Custom
Malware Detection	Moskovitch [114]	2008	✗	✓	✗	◐	✓	✓	✗	Custom
	Santos [115]	2011	✗	✗	✓	✗	✓	✓	◐	Custom
	Nissim [116]	2012	✗	◐	✓	◐	✗	✗	✗	Private
	Zhao [117]	2012	✗	✗	✗	✗	✓	✓	◐	Private
	Nissim [118]	2014	✓	✓	✗	◐	✓	✓	✗	Custom
	Zhang[119]	2015	◐	◐	✗	✗	✓	✓	✗	Private
	Nissim [120]	2016	✗	✓	✓	◐	✓	✓	◐	Custom
	Ni [121]	2016	✓	✓	✗	◐	✓	✓	◐	Private
	Chen [122]	2017	✓	✓	✗	◐	✗	✗	◐	Private
	Rashidi [66]	2017	✗	✓	✓	◐	✓	✓	✗	Drebin
	Fu [123]	2019	✓	✓	✗	✗	✓	✗	◐	Private
	Irofti [124]	2019	◐	◐	✗	◐	✗	✗	✓	DREBIN, EMBER
	Pendlebury [86]	2019	✗	✗	✓	◐	✓	✓	✓	AndroZoo
	Sharmeen [125]	2020	✓	◐	✗	◐	✓	✓	◐	Drebin, AndroZoo
	Chen [126]	2020	◐	◐	✓	✗	✓	✓	◐	MCC
	Koza [11]	2020	✓	◐	✓	◐	✓	✗	✓	Private
	Noorbehbahani [13]	2020	✓	✗	✗	◐	✓	✓	✗	AndMal17
	Li [127]	2021	✗	◐	✗	◐	✓	✗	◐	FalDroid, DREBIN, Genome
	Liang [109]	2021	✓	◐	✓	◐	✓	✓	◐	Custom

- Req. 4 we use ◐ if only some 'cross-validation' is performed, ✓ if statistical comparisons are made or mentioned, and ✗ if no form of verification is mentioned.
- For Req. 5, we report two columns: '*Labels*' denotes whether the provided information allows to determine the actual number of labelled samples used to train and test all the considered models; whereas '*Balance*' denotes whether the balancing ratios are clearly specified.
- For Req. 6, ✗ denotes if the provided information is insufficient for reproduction; ✓ if the source code is open; and ◐ if only intermediate information is provided.

In the last column we report the datasets used in each paper: here, 'Private' means that the data was never made available, whereas 'Custom' means that it was composed in-house via public sources, but that the actual samples cannot be recovered (i.e., it is not possible to retrieve the public feeds of past years).

4.2. Findings

By observing Table 1, we derive the following.

1) No one fits all, because no paper meets all requirements.
2) Few compare their SsL methods with a lower bound.
3) Worst case scenarios are rarely covered.
4) Lack of statistically significant comparisons, preventing any certification of the final results.
5) Poor reproducibility and limited datasets, which is a known trend in ML research [128].

Although no paper meets all our requirements, there are some good efforts. Remarkably, Zhao et al. [111] meet almost all requirements (with the exception of a single dataset, and their implementation not being available today), and are the only ones to mention a statistical comparison via a student t-test; however, we were not able to infer how the starting dataset was split in training and testing. We also praise the work in [11], but it lacks a vanilla $\underline{SsL}$ for ablation studies (due to fine tuning of confidence thresholds), and only a limited cross-validation is performed. Noteworthy is also [109], whose authors fairly evaluate different SsL techniques (although none of these can be considered as an ablation study) for two CTD tasks (NID and MD), but each on a single dataset.

The situation portrayed by Table 1 does not imply that all past works are wrong or flawed: these papers are published in high quality venues, and we acknowledge their significance. On the contrary, the true message of Table 1 is highlighting the *immaturity* of the state-of-the-art with respect to realistic deployments of SsL. No attention has been given to systematic assessments of the benefits provided by unlabelled data in SsL.

The case of active learning. We observe that many papers in Table 1 use active learning methods, most of which in lifelong learning settings. In these cases, considering a model trained via random draws from $\mathbb{U}$ (instead of 'active' suggestions) can simultaneously meet both Req. 1 and 2. This is notably done by Gornitz

et al. [95] (despite not meeting Req. 3). In contrast, Pendlebury et al. [86] apply active learning by labelling *all* samples with confidence below 1%, which results in 700 samples, and the improvement is shown against a model that does not make use of any additional label, leading to an unfair comparison. The evaluation protocol of these and similar papers is, however, *legitimate*. They operate under the assumption that the ML model is already trained and deployed, meaning that unlabelled data will naturally occur. In such conditions, the focus is not on "determining the benefits of unlabelled data for ML deployment" (which is our focus), but rather on "how to maximize the performance of an existing ML system with additional unlabelled data streams". Both [86] and [95] achieve that. Nonetheless, to the best of our knowledge (semi)*supervised* ML systems are not widely deployed (yet) in CTD, demanding further investigations of their potential benefits *in advance*.

Relationship with other domains. There are several studies that expose evaluation issues of ML methods, and Dehgani et al. [129] invite devising specific guidelines. However, within the context of SsL, existing proposals are *not applicable* to CTD. For instance, Oliver et al. [16] suggest transferring models between different datasets: this may not be feasible for CTD because datasets contain divergent feature sets and model transferring can be a recommendation at best, and not a requirement. Similarly, [130] mention random sampling, but do not emphasize the statistical significance which is crucial for SsL in CTD due to the huge search space to extract a small $\mathbb{L}$ from a huge $\mathbb{D}$. This is less of a problem in, e.g., Computer Vision, where most datasets (e.g., CIFAR) have been used thousands of times and benchmarks results are well-known; moreover, the corresponding community is more open to source code disclosure. Because of these reasons, it is crucial to establish a specific set of requirements for CTD applications of SsL.

Regardless, some of our requirements are not met also by relevant works. An exemplary case, which exploits data augmentation in CIFAR, is MixMatch [20]. Here, no lower bound SL is considered: as a matter of fact, they only report the results of the upper bound $\overline{SL}$ trained on 50K samples (i.e., most of CIFAR). We do acknowledge that CIFAR is well-known and performance on small subsets can be easily assessed, but a fair comparison requires to evaluate such performance by using the same settings (i.e., same $\mathbb{L}$ and same classifier).

Takeaway: the current state-of-the-art does not allow to assess the benefits of SsL methods. Such immaturity is due to the lack of a rigorous evaluation protocol for SsL methods in CTD.

5. Proposed Evaluation Framework

As a constructive step forward, we present CEF-SsL, an original Cybersecurity Evaluation Framework for SsL, which meets all the requirements in §3.3.

CEF-SsL aims to provide a practical assessment of SsL methods by using any fully labelled dataset, while simultaneously considering the deployment budget $\mathcal{B}$ and ensuring the statistical significance of the results. Because $\mathbb{U}$ can be easily obtained, CEF-SsL assumes that $\mathcal{U}$ is fixed and, hence, plays no role in practical comparisons. CEF-SsL has four *inputs*:

- $\mathbb{D}$ represents a large and fully labelled dataset. Such $\mathbb{D}$ can be either: (i) openly accessible; or (ii) created ad-hoc via simulations, well-known security feeds, or by manually labelling real data. CEF-SsL assumes that the labels in $\mathbb{D}$ are verified, i.e., all samples have the correct ground truth, which is the typical assumption in ML research. CEF-SsL uses $\mathbb{D}$ as basis[14] to compose the four datasets required for a practical evaluation $\mathbb{L}$, $\overline{\mathbb{L}}$, $\mathbb{U}$, and $\mathbb{F}$.
- $\mathcal{L}$ is the labelling budget which is used to to compose $\mathbb{L}$ (cf Eq. 1). CEF-SsL assumes that $\mathcal{L}$ is fixed for the entire simulation. Variations of $\mathcal{L}$ imply different scenarios (hence, different $\mathbb{L}$) which lead to unfair comparisons among models. If necessary, CEF-SsL can be applied again on different values of $\mathcal{L}$.
- $\overrightarrow{\text{ML}}$ denotes an *array of ML methods*. Such array must contain the specifics to devise all the baseline models (SL, $\overline{SL}$, $\underline{SsL}$) plus any additional model that should be included in the evaluation. All the resulting models will be developed on the same labelling budget $\mathcal{L}$.
- (n, k) is a pair of integers that regulate the 'runs' of CEF-SsL to achieve statistically significant results.

The *output* are two $(n \cdot k)$-dimensional arrays, whose elements include the results of all the models devised by following $\overrightarrow{\text{ML}}$ on each run, specifically: $\overrightarrow{\mu}$, containing the performance on 'assumed' future data, and $\overrightarrow{\varepsilon}$ containing any cost incurred during the development (not related to labelling).

We provide an overview of CEF-SsL in Fig. 4. CEF-SsL can be divided in three stages: Prepare, Run, Iterate.

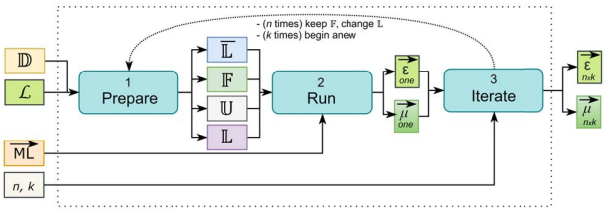

Figure 4: CEF-SsL. The $\mathcal{L}$ can also be provided as input for the second stage.

5.1. Stage one: Prepare

The first stage uses $\mathcal{L}$ to partition $\mathbb{D}$ into $\mathbb{L}$, $\overline{\mathbb{L}}$, $\mathbb{U}$, and $\mathbb{F}$. Fig. 5 shows a schematic representation of such workflow.

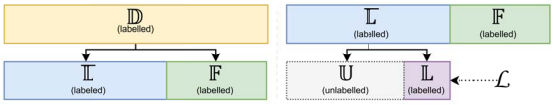

Figure 5: $\mathbb{D}$ is first split into $\mathbb{F}$ and $\overline{\mathbb{L}}$. Then $\overline{\mathbb{L}}$ is further split into $\mathbb{L}$ according to $\mathcal{L}$, and the remaining samples are considered as unlabelled $\mathbb{U}$.

14. $\mathbb{D}$ is assumed to be already preprocessed, and it can be a subset of an existing dataset, but the selection must be unbiased.

CEF-SsL begins by splitting $\mathbb{D}$ in $\mathbb{F}$ and $\overline{\mathbb{L}}$: the former, $\mathbb{F}$, is used exclusively to assess the performance on future data[15]; the latter, $\overline{\mathbb{L}}$ is used for all remaining 'training' operations, because $\overline{\mathbb{L}}$ can serve as basis to generate $\mathbb{L}$, and then treat the remaining samples as unlabelled, representing $\mathbb{U}$.

Generating $\mathbb{F}$ from $\mathbb{D}$ depends on the considered CTD task. The selection is done so as to achieve a representative $|\mathbb{F}|$ and $\rho(\mathbb{F})$, while ensuring that the left-out samples (which will represent $\overline{\mathbb{L}}$) allow to create meaningful $\mathbb{L}$ and $\mathbb{U}$. Such selection can also take into account the temporal relationships (if available) among the samples in $\mathbb{D}$. For example, $\mathbb{F}$ can be composed by selecting only the 'most recent' samples in $\mathbb{D}$, allowing assessment of potential concept drift [24].

To generate $\mathbb{L}$ from $\overline{\mathbb{L}}$, we recall that $\mathcal{L} = \sum_{x \in \mathbb{L}} \mathcal{C}_x$. Therefore, CEF-SsL chooses samples from $\overline{\mathbb{L}}$ and assigns them to $\mathbb{L}$, each time by decreasing the labelling budget $\mathcal{L}$ according to the cost of each sample[16]. However, $\mathbb{L}$ must include at least some benign and malicious samples. To this purpose, CEF-SsL requires a *minimum* amount of samples for each class. CEF-SsL will then populate $\mathbb{L}$ by randomly sampling as many samples of that class from $\overline{\mathbb{L}}$ (while decreasing the labelling budget accordingly); then, CEF-SsL will use the remaining budget to further populate $\mathbb{L}$ randomly. We observe that by setting different labelling costs $\mathcal{C}_x$ it is possible to simulate imbalanced data distributions: we will showcase such intriguing property of CEF-SsL in our demonstration. At this point, CEF-SsL will consider all the samples in $\overline{\mathbb{L}}$ not included in $\mathbb{L}$ as unlabelled, representing $\mathbb{U}$. The case where one (or many) SsL approaches in $\overrightarrow{\text{ML}}$ involve the usage of exploratory techniques is covered in the following stage.

5.2. Stage two: Run

The second stage begins with Reqs. 1–3. Specifically:

1) train SL on $\mathbb{L}$ and test it on $\mathbb{F}$ as $\mu(SL)$; account for all operational costs as $\varepsilon(SL)$;
2) train $\overline{SL}$ on $\overline{\mathbb{L}}$ and test it on $\mathbb{F}$ as $\mu(\overline{SL})$; account for all operational costs as $\varepsilon(\overline{SL})$.
3) use $\mathbb{L}$ and $\mathbb{U}$ to devise $\underline{SsL}$, and test it on $\mathbb{F}$ as $\mu(\underline{SsL})$; account for all operational costs as $\varepsilon(\underline{SsL})$.

Then, CEF-SsL focuses on each remaining method in $\overrightarrow{\text{ML}}$:

- if the SsL method does not make any assumptions on $\mathbb{L}$, then CEF-SsL uses $\mathbb{U}$ and the previously drawn $\mathbb{L}$ as input for the SsL method.
- if the SsL method requires $\mathbb{L}$ to be composed in a more refined way, then CEF-SsL generates a new $\mathbb{L}$ according to the specifics of the SsL method. The cost of labelling is 'charged' to $\mathcal{L}$ and all other costs are accounted as $\varepsilon(SsL)$. The resulting $\mathbb{L}$ and (new) $\mathbb{U}$ are then used as input to the SsL method.
- Finally, the respective SsL model is trained, and tested on $\mathbb{F}$ resulting in $\mu(SsL)$; all the operational costs are accounted in $\varepsilon(SsL)$.

At the end of this stage, CEF-SsL populates the respective $\overrightarrow{\mu}$ and $\overrightarrow{\varepsilon}$ with the specific performance and (extra) costs of all the considered models of this single 'run'.

15. $\mathbb{F}$ has no relationship with the labelling budget $\mathcal{L}$ and $\mathbb{F} \cap (\mathbb{U} \cup \mathbb{L}) = \varnothing$.

16. Such cost can be fixed, or can vary depending on the desired level of realistic fidelity by associating each sample $x \in \mathbb{D}$ with a custom $\mathcal{C}_x$.

5.3. Stage three: Iterate

To obtain statistically significant results, CEF-SsL performs multiple 'runs', according to the iteration parameters (n, k) provided as input. Specifically:

- CEF-SsL repeats its entire workflow k times, each time by choosing a new $\mathbb{F}$, leading to different $\overline{\mathbb{L}}$ and, hence, different $\mathbb{L}$ and $\mathbb{U}$.
- For each (new) $\mathbb{F}$, CEF-SsL composes a different $\mathbb{L}$ (and, hence, different $\mathbb{U}$) for n times to account for randomness.

Altogether, CEF-SsL will evaluate *each method* in $\overrightarrow{\text{ML}}$ a total of $n \cdot k$ times, resulting in as many μ and ε, all of which will be inserted into $\overrightarrow{\mu}$ and $\overrightarrow{\varepsilon}$. To assess different $\mathcal{L}$, CEF-SsL can be launched again by maintaining all the other inputs.

Finally, the aggregated results of each method can be validated via, e.g., a Student t-test [131] or the more refined Wilcoxon Ranksum test [132]—provided that CEF-SsL is run enough times to provide statistically significant results (e.g., 50s or more [133]). Such comparisons can be made by considering different initial conditions (e.g., multiple values of $\mathcal{L}$), because CEF-SsL ensures that all such conditions are shared across all methods: hence, the only difference is which ML method produced each single result.

6. Demonstration

As a final contribution of this SoK paper, we demonstrate the application of our CEF-SsL framework to assess the benefits of SsL in CTD. We do so via a comprehensive set of experiments on 9 well-known datasets, where we consider 9 existing SsL methods. Such demonstration aims to:

- showcase the application of our cost model and CEF-SsL;
- further motivate the importance of our requirements;
- provide the first statistically validated *benchmark* for future studies.

Moreover, all the 9 considered datasets are publicly available, and we release the code of our CEF-SsL implementation[17].

We first outline the considered datasets (§6.1). Next, we explain the considered SsL methods (§6.2) and their implementation through CEF-SsL (§6.3). We then summarize the results (§6.4) and showcase a statistically significant comparison (§6.5). We report in the Appendix some low-level technicalities (§A) and the full benchmark results (§B).

6.1. Datasets

Our evaluation focuses on the three CTD areas considered in this paper (§2): NID, PWD, MD. For each area we consider three publicly available datasets.

For NID, we use: `CTU13`, `UNB15`, `IDS17`. These datasets are well-known in the NID community, and contain network data representing a mixture of simulated and real traffic of large networks. `CTU13` is provided as PCAP traces

17. Available at: https://github.com/hihey54/CEF-SsL

and is focused on *botnet* detection; UNB15 and IDS17 are provided as NetFlows and contain additional malicious activities such as DoS, exploits, or reconnaissance operations.

For PWD, we use: UCI, δPhish, Mendeley. These well-known datasets contain information on webpages, such as the URL, the reputation of the website, and the contents of the source HTML. Two (UCI and Mendeley) are provided directly as features, while δPhish has raw webpages, from which we extract the features by following established practices [134].

For MD, we use: Drebin, Ember, AndMal20. These datasets are widely employed for ML-related analyses on malware targeting different OS: Ember for Windows, Drebin and AndMal20 for Android. Although Drebin is becoming outdated (it was collected in 2013), AndMal20 is very recent and serves for a better representation of current trends.

After obtaining all these 9 datasets, we preprocess them so that they are usable for our objectives. For instance, we clean some redundant data, or derive their feature sets. Some datasets may contain samples of different malicious classes. Because our focus is on *detection*, in some cases (Drebin, AndMal20) we aggregate all of them into a single malicious class. Datasets for PWD and Ember only have one malicious class. Datasets for NID have a huge variety: as done in previous work [40], we consider one classifier per each specific attack. More details are in the Appendix A.1. Regardless, all these operations are fixed for all the ML models evaluated on each dataset, meaning that their impact on ε is the same for each model and, hence, negligible for comparisons.

We provide an overview of these datasets after all preprocessing has taken place in Table 2. For each dataset $\mathbb{D}$, we report the overall amount of benign and malicious samples ($\mathbb{D}_b$ and $\mathbb{D}_m$, respectively), the amount of malicious classes (N), the reiterations (n, k) performed by CEF-SsL, and reference to a past work that used such dataset (SotA).

TABLE 2: Considered Datasets

CTD	Name	$\mathbb{D}_b$	$\mathbb{D}_m$	N	(n,k)	SotA
NID	CTU13 [44]	19.5M	444K	6	(11,3)	[135]
	UNB15 [45]	100K	2.22M	4	(23,4)	[136]
	IDS17 [43]	555K	2.21M	5	(15,3)	[137]
PWD	UCI [138]	4898	6157	1	(20,5)	[139]
	Mendeley [140]	58K	31K	1	(20,5)	[141]
	δPhish [50]	5510	1013	1	(20,5)	[50]
MD	Drebin [142]	123K	4022	1	(20,5)	[143]
	Ember [144]	400K	400K	1	(20,5)	[145]
	AndMal20 [146]	162K	195K	1	(20,5)	[147]

For each dataset, CEF-SsL performs all experiments N times, totalling N$*(n*k)$ runs.

6.2. Selected SsL Methods

Let us describe the SsL methods that are included in $\overrightarrow{ML}$ in out study, together with the two SL baselines. Evaluation of all SsL methods proposed in the state-of-the-art (cf. Table 1) is clearly infeasible and also inpossible due to their limited reproducibility and different assumptions. To showcase all scenarios envisioned in our CEF-SsL framework, we consider 9 SsL methods which are variations of two established SsL methods: *self learning via pseudo-labelling* (e.g., [65]) and *active learning via uncertainty sampling* (e.g., [66]), summarized in §2.3. Specifically, we consider 3 'pure' pseudo-labelling methods, 3 'pure' active learning methods, and 3 combinations thereof (e.g., [70]), where we cascade pseudo-labelling with active learning. The decision criterion is the *confidence* threshold c.

Pseudo Labelling. One of the 'pure' pseudo labelling models represents our SsL baseline. Specifically, we devise:

- SsL, using all pseudo labels regardless of their confidence; the process is entirely automated because $\mathbb{L}$ is chosen randomly and no selection of c is required.
- $\pi\, SsL$, using only the pseudo labels with the highest confidence $c \geq 99\%$;
- $\widehat{\pi}\, SsL$, which repeats the previous operation another time. We use $\pi\, SsL$ to predict the remaining $\mathbb{U}$, and insert the corresponding pseudo-labelled samples with $c \geq 99\%$ in the 'mixed' $\mathbb{L}$.

Active Learning. For these methods, we assume that half of the labelling budget is used initially to develop the first learner, and then the remaining half is used to randomly assign the correct label (according to the source dataset) to those samples that meet a specific confidence threshold. Due to randomness, we repeat the draw 5 times for each active learning method. Depending on c, we consider:

- $\alpha\, SsL_l$ by drawing from low confidence samples $c \leq 1\%$;
- $\alpha\, SsL_h$ by drawing from high confidence samples $c \geq 99\%$;
- $\alpha\, SsL_o$ by drawing from the other samples $1\% < c < 99\%$;

We note that our implementation of active learning is fundamentally different and more realistic than the one adopted by Pendlebury et al. [86]: in Tesseract, the oracle assigns the correct label to *all* samples within a certain confidence; on the other hand, we simply use the learner to provide a set of samples to the oracle, who can only label as many samples as allowed by the remaining budget. This ensures that the provided $\mathcal{L}$ is *never* exceeded, allowing for fair comparisons.

Pseudo-Active Learning. We combine pseudo labelling with active learning by using $\pi\, SsL$ as initial learner (but developed to use half of the initial $\mathcal{L}$), which is used to produce three 'pseudo-active' methods ($\alpha^{\pi} SsL_l$, $\alpha^{\pi} SsL_o$, $\alpha^{\pi} SsL_h$) in the same way as in the 'pure' active learning.

6.3. Implementation

We now describe our implementation of CEF-SsL, which performs the same operations for all considered $\mathbb{D}$ and $\overrightarrow{ML}$.

The first step of CEF-SsL is the creation of $\mathbb{F}$ from $\mathbb{D}$. In our case, we do so by adopting the 80:20 split which is common in CTD (e.g., [40], [148], [149]). Specifically, CEF-SsL randomly chooses 20% of the malicious samples in $\mathbb{D}$ and 20% of the benign samples in $\mathbb{D}$, and puts them into $\mathbb{F}$. The resulting samples are then considered as $\overline{\mathbb{L}}$.

To allow a comprehensive benchmark, we consider three scenarios where the cost of labelling each sample varies depending on their class—which serves to investigate different *balance ratios* $\rho(\mathbb{L})$. Specifically:

- (balanced) $\mathcal{C}_m = \mathcal{C}_b$, where the # of benign samples matches the # of malicious samples, $\rho(\mathbb{L}) = (50, 50)$;
- (unbalanced) $\mathcal{C}_m = 2 \cdot \mathcal{C}_b$, where the # of benign samples is twice the # of malicious samples, $\rho(\mathbb{L}) = (66, 33)$;
- (very unbalanced) $\mathcal{C}_m = 5 \cdot \mathcal{C}_b$, where # of benign samples is five times the # malicious samples, $\rho(\mathbb{L}) = (84, 16)$.

Where b and m denote a benign and malicious sample, respectively. For each cost scenario, we vary the allocated labelling budget $\mathcal{L}$ four times. We do so by regulating the minimal amount of *benign* samples, $\mathbb{L}_b$, to be included in $\mathbb{L}$. Hence, CEF-SsL composes $\mathbb{L}$ by first selecting $\mathbb{L}_b$ benign samples from $\overline{\mathbb{L}}$; then, CEF-SsL keeps populating $\mathbb{L}$ by choosing malicious samples from $\overline{\mathbb{L}}$ until the budget $\mathcal{L}$ has completely run out, resulting in $\mathbb{L}_m$ malicious samples. The values of $\mathcal{L}$ and $\mathbb{L}_b$ depend on each CTD task, and are reported in Table 3. Because each combination of $\mathcal{L}$ and $\mathcal{C}$ represents a different setting, we restart CEF-SsL at each change (hence, 12 times) to allow a fair comparison.

TABLE 3: Composition of $\mathbb{L}$ for different $\mathcal{L}$ and $\mathcal{C}$. In all cases, $|\mathbb{L}|$=($\mathbb{L}_m$+$\mathbb{L}_b$), $\mathbb{F}$=0.2*$\mathbb{D}$, $\overline{\mathbb{L}}$=0.8*$\mathbb{D}$, and $\mathbb{U}$=($\overline{\mathbb{L}}$-$\mathbb{L}$).

CTD	NID			PWD			MD		
Scenario and $\mathcal{C}$	$\mathcal{L}$	$\mathbb{L}_m$	$\mathbb{L}_b$	$\mathcal{L}$	$\mathbb{L}_m$	$\mathbb{L}_b$	$\mathcal{L}$	$\mathbb{L}_m$	$\mathbb{L}_b$
balanced $\mathcal{C}_b = \mathcal{C}_m$	100	50	50	40	20	20	80	40	40
	200	100	100	80	40	40	160	80	80
	400	200	200	160	80	80	320	160	160
	800	400	400	320	160	160	640	320	320
unbalanced $\mathcal{C}_m = 2 * \mathcal{C}_b$	200	50	100	80	20	40	160	40	80
	400	100	200	160	40	80	320	80	160
	800	200	400	320	80	160	640	160	320
	1600	400	800	640	160	320	1280	320	640
very unbalanced $\mathcal{C}_m = 5 * \mathcal{C}_b$	500	50	250	200	20	100	400	40	200
	1000	100	500	400	40	200	800	80	400
	2000	200	1000	800	80	400	1600	160	800
	4000	400	2000	1600	160	800	3200	320	1600

We observe that our choices of $\mathcal{L}$ result in $\mathbb{L}$ that are *smaller* than the testing set $\mathbb{F}$, which is a good practice in CTD research [54]. Overall, our models are trained with as little as 40 labels (for PWD), and as high as 2400 labels (for NID) The resulting sets $\overline{\mathbb{L}}$ and $\mathbb{L}$ are immediately used to train the lower bound SL and the upper bound $\overline{SL}$, both tested on $\mathbb{F}$. Then, CEF-SsL uses the remaining sets according to each SsL method in $\overrightarrow{ML}$. More detailed information on such development can be found in Appendix A.2.

6.4. Evaluation

We apply the described implementation of CEF-SsL on each dataset. The considered ML methods use the Random Forest (RF) learning algorithm, for three reasons. First, because RF are widely adopted by past work (e.g., [40], [86], [143], [145]), favoring comparisons. Second, since RF are known to provide an excellent tradeoff between performance and computation time, and they can also be parallelized: to provide statistically significant results we must consider thousands of models, hence we favor algorithms that are fast to train. Third, because preliminary analyses confirmed the previous statement: we empirically found that RF achieve similar performance as other algorithms (e.g., neural networks) while requiring a fraction of the training time.[18]

18. We do not aim at benchmarking every conceivable implementation of SsL methods. Nevertheless, our CEF-SsL code allows to select a different learning algorithm by changing just one line of code.

Performance Assessment. We choose the *F1-score* (a positive is a malicious sample) as performance metric, which is common in CTD.[19] We report in Table 4 the *average* F1-score achieved by each method in $\overrightarrow{ML}$ on each dataset, across all the different combinations of $\mathcal{L}$ and $\mathcal{C}$. More granular analyses that consider model-to-model comparisons can be made by looking at the full results in Appendix B.

TABLE 4: Average F1-score of all methods. We denote in bold the best SsL method on each dataset. Cells in gray denote the best 'pure' pseudo labelling method, while a dark gray denotes the best active learning method.

CTD	NID			PWD			MD		
Method	CTU13	UNB15	IDS17	Mend	UCI	δPhish	DREBIN	Ember	AndMal
$\overline{SL}$	0.979	0.942	0.989	0.958	0.974	0.958	0.907	0.970	0.986
SL	0.611	0.447	0.878	0.852	0.884	0.780	0.480	0.667	0.910
$\underline{SsL}$	0.613	0.447	0.879	0.852	0.886	**0.778**	0.486	0.662	0.910
$\pi\ SsL$	0.588	0.437	0.820	0.850	0.884	0.778	0.474	0.647	0.900
$\widehat{\pi}\ SsL$	0.584	0.435	0.818	0.849	0.883	0.777	0.470	0.641	0.890
$\alpha\ SsL_l$	**0.693**	0.582	**0.897**	**0.863**	**0.903**	0.770	**0.546**	**0.687**	**0.924**
$\alpha\ SsL_o$	0.637	0.577	0.874	0.855	0.891	0.745	0.497	0.673	0.916
$\alpha\ SsL_h$	0.510	0.436	0.786	0.834	0.851	0.714	0.423	0.598	0.892
$\alpha^{\pi} SsL_l$	0.664	0.533	0.853	0.861	0.901	0.767	0.529	0.654	0.901
$\alpha^{\pi} SsL_o$	0.633	**0.595**	0.857	0.854	0.890	0.745	0.489	0.647	0.895
$\alpha^{\pi} SsL_h$	0.486	0.427	0.744	0.833	0.851	0.711	0.410	0.579	0.865

The following insights can be drawn from Table 4. First, albeit almost counter-intuitive, using *all* pseudo-labels is the most effective among the 'pure' pseudo labelling techniques. Second, despite the identical labelling budgets in NID datasets, SsL methods achieved varying performance: in UNB15 they achieve only 0.6 F1-score at best, whereas in IDS17 they can reach almost 0.9 F1-score; this highlights the importance of conducting evaluations on diverse datasets. Third, active learning appears to be the best way to use the labelling budget, but in δPhish it is always inferior to 'pure' pseudo labelling; moreover, it is interesting that the results of the models trained on the (correct) high confidence labels consistently achieve the worst performance. Fourth, in all datasets, all models performed very similarly (on average) to the baseline SL. Such small gap requires to be further investigated via statistical comparisons, which we will do in §6.5.

Assessment of Extra Costs. Many factors contribute to ε for each considered ML method. All of our implemented methods share the same testbed, and most of such costs are equal for all methods. We hence focus on the most salient 'cost' of each method that we can measure: its *execution time*.

We report in Table 5 the total time required to develop each model, which comprises all the steps for (re)training and (for SsL methods) predicting unlabelled data.

TABLE 5: Average execution time (seconds) of all methods. Bold values denote the SsL method with best F1-score on the same dataset (cf. Table 4).

CTD	NID			PWD			MD		
Method	CTU13	UNB15	IDS17	Mend	UCI	δPhish	DREBIN	Ember	AndMal
$\overline{SL}$	30.31	18.75	33.55	1.365	0.420	0.535	3.054	147.6	42.81
SL	0.392	0.388	0.393	0.349	0.390	0.401	0.381	0.395	0.438
$\underline{SsL}$	35.00	24.44	39.65	1.199	1.036	**1.040**	1.430	101.4	30.53
$\pi\ SsL$	12.74	15.32	23.92	1.090	0.930	0.942	1.064	2.257	3.702
$\widehat{\pi}\ SsL$	27.00	28.77	45.13	1.864	1.473	1.487	1.824	6.791	8.726
$\alpha\ SsL_l$	**3.471**	4.955	**8.990**	**0.905**	**0.885**	0.895	**0.847**	**0.897**	**0.960**
$\alpha\ SsL_o$	3.469	4.954	8.989	0.904	0.883	0.896	0.846	0.895	0.957
$\alpha\ SsL_h$	3.466	4.950	8.987	0.898	0.880	0.894	0.844	0.893	0.952
$\alpha^{\pi} SsL_l$	23.49	27.22	38.50	1.744	1.356	1.375	1.666	5.267	7.593
$\alpha^{\pi} SsL_o$	23.39	**26.98**	38.48	1.746	1.354	1.375	1.662	5.493	7.699
$\alpha^{\pi} SsL_h$	23.28	26.78	38.06	1.747	1.350	1.372	1.655	5.258	7.579

19. We also measure Recall and Precision, reported in our GitHub repository.

From Table 5, we can observe that the model requiring the highest time is often the baseline $\underline{SsL}$. This is not surprising, because it is trained on the *entire* $\mathbb{U}$ after training the baseline SL, and using it to predict the entire $\mathbb{U}$. In contrast, all other models are trained on a much smaller dataset.

However, using only the *execution* time when comparing the ε is not always fair. Some models may be better in terms of execution time but require some manual tuning, e.g., setting the desired level of confidence c. Compare, for instance, $\underline{SsL}$ and $\alpha\,SsL_l$ on CTU13: the former requires 35s, whereas the latter only 3s, which is a 32s difference. However, choosing an appropriate c for $\alpha\,SsL_l$ requires: (i) inspecting the results of $\alpha\,SsL_l$, (ii) setting the new c, (iii) devising a new $\alpha\,SsL_l$, (iv) inspecting the results of the new $\alpha\,SsL_l$, and (v) deciding whether it has acceptable performance or not. These procedures have a human in the loop and hence a significantly higher ε (which cannot be shown in Table 5). On the other hand, $\underline{SsL}$ *always* achieves the reported performance, and by being entirely automated will result in an overall lower ε.

6.5. Statistical Validation

To substantiate the claim that some SsL using $\mathbb{U}$ outperforms the respective baseline (SL or $\underline{SsL}$), statistical tests can be carried out. Here, we use the Wilcoxon ranksum [132], in which two populations are compared with the goal of verifying a given null hypothesis H_0. The test outputs a z-value used to derive a p-value: H_0 can be accepted or rejected on the basis of such p, according to a target significance level. We use the two-tailed version of the test, hence our H_0 is that the two populations are statistically equivalent: the larger the p-value, the more H_0 should be accepted (and viceversa). We set the significance level to 0.05, implying that if $p > 0.05$ then the two populations are equivalent; conversely, if $p \leq 0.05$, the two populations are different (this is especially true if $p \ll 0.05$).

For each dataset, we compare the populations containing the performance of the baseline SL against: (i) the best 'pure' pseudo-labelling method (gray cells in Table 4); and (ii) the best active learning method (dark gray cells in Table 4). We are comparing[20] the *methods*, not the individual *models* (model-to-model comparisons can be made from Figs. 6–8). The results of such tests are in Table 6, reporting the size of the populations[21], and the output z- and p values.[22]

From Table 6, we can draw the following conclusions.

Active Learning provides **statistically significant improvements**, which can be remarkable (cf. Figs 6–8); a finding that is consistent with past works (e.g., [95]). However, this is not always true: on IDS17, $\alpha\,SsL_l$ is statistically equivalent to SL, meaning that there is *no* benefit in using $\mathbb{U}$ on IDS17 (at least according to our testbed). Moreover, it can be *detrimental*: on δPhish, the best method using active learning ($\alpha\,SsL_l$) yields lower performance than the baseline SL, and such difference is statistically significant (p=0.002$\ll$0.05).

Pseudo Labelling **is not useless**. In UNB15, the pseudo-active method $\alpha^{\pi}SsL_o$ statistically outperforms the baselines (SL, and also $\underline{SsL}$). However, in all its 'pure' applications, it provides no benefit: its best performer is $\underline{SsL}$, which is *always* statistically equivalent to SL. To put it differently, in the 'worst case' using $\mathbb{U}$ will not induce performance loss.

Finally, we also conducted the one-tailed variant of the statistical test, which confirms all previous findings.

TABLE 6: We statistically compare the SL baseline method against the best 'pure' pseudo-labelling and the best active learning methods. Bold values denote when H_0 is accepted ($p > 0.05$), i.e., the two methods are statistically equivalent. Cells in green (red) denote cases where using $\mathbb{U}$ statistically increases (decreases) performance.

		Best 'pure' pseudo-labelling			Best active learning		
Dataset	PopSize	Method	p-value	z-value	Method	p-value	z-value
CTU13	396	$\underline{SsL}$	**0.873**	0.159	$\alpha\,SsL_l$	< 0.001	4.310
UNB15	1104	$\underline{SsL}$	**0.964**	–0.044	$\alpha^{\pi}SsL_o$	< 0.001	15.98
IDS17	540	$\underline{SsL}$	**0.932**	0.085	$\alpha\,SsL_l$	**0.978**	–0.027
UCI	1200	$\underline{SsL}$	**0.473**	0.717	$\alpha\,SsL_l$	< 0.001	7.386
Mend.	1200	$\underline{SsL}$	**0.713**	0.368	$\alpha\,SsL_l$	< 0.001	6.757
δPhish	1200	$\underline{SsL}$	**0.554**	–0.590	$\alpha\,SsL_l$	0.002	–3.113
Drebin	1200	$\underline{SsL}$	**0.310**	1.015	$\alpha\,SsL_l$	< 0.001	11.78
Ember	1200	$\underline{SsL}$	**0.603**	–0.512	$\alpha\,SsL_l$	< 0.001	3.407
AndMal	1200	$\underline{SsL}$	**0.712**	–0.370	$\alpha\,SsL_l$	< 0.001	12.01

7. Discussion and Future Work

Let us finalize our evaluation with some crucial remarks.

Importance of our Requirements. Without considering SL, it was not possible to determine that any 'pure' pseudo-labelling model was not just useless but even detrimental, due to achieving the same or inferior $\mu(\cdot)$ while requiring higher $\mathcal{B}$. For instance, consider the detailed results on UCI in Fig. 7a: the SsL models achieve a respectable F1-score of 0.9 when trained only on 40 labelled examples. However, the same result is achieved by the baseline SL, which does not make use of an $\mathbb{U}$ containing 8000 samples. Similarly, on AndMal20, investing in $\mathcal{U}$ provides very little benefit because the performance gap between SL and $\overline{SL}$ is marginal. Furthermore, active learning was considered to be superior to random sampling [12], but for two of our datasets, IDS17 and δPhish, this cannot be confirmed. Such insights would not have been possible without a massive and statistically validated comparison: looking only at Table 4, one may conclude that the best active learning model has better average performance than the SL baseline. Finally, by considering Req. 2, it was possible to determine the lowest *cost* induced by using $\mathbb{U}$ in the SsL pipeline due to lack of human supervision (cf. Table 5).

Balancing. An intriguing occurrence can be observed from Figs. 6–8. In the presence of data-imbalance, the performance can be *lower* despite a *higher* labelling budget. This is evident for Ember (Fig. 8b). In the balanced scenario where $\mathcal{C}_m$=$\mathcal{C}_b$ (leftmost plot): when $\mathbb{L}$ contains 800 correct labels, all models converge to a 0.8 F1-score; however, when $\mathcal{C}_m$=5$\mathcal{C}_b$ (rightmost plot), the performance when $\mathbb{L}$ has 2400 correct labels ranges from 0.55 to 0.75 F1-score. We tried to regulate these situations by applying oversampling techniques (e.g., [150]), but we never saw

20. The test is valid: the compared populations have the same amount of elements and the conditions are shared among all elements, where the only difference is the generation process (i.e., the specific ML method).

21. Such size is given by n*k*12, because we consider 3 cost scenarios with 4 budgets. For NID, each element is the average of the N malicious classes.

22. The *EffectSize* of the test can be dervied by $\frac{z}{\sqrt{\text{PopSize}}}$.

significant changes. Such interesting result also occurs on AndMal20 and UCI despite at a lower magnitude.

Scope. Despite our extensive evaluation, we stress that our results should serve as a basis for future works, and should not be used to derive 'universal' statements. For instance, the considered SsL methods represent just a subset of all conceivable SsL techniques: hence our experiments cannot be used to conclude that "all pseudo-labelling techniques are not very effective in CTD". In addition, we stress that we apply well-known methods on existing datasets and do not claim superiority over past works. In Appendix C, we present a case study comparing our results with a recent paper [70] that uses a similar testbed as ours. Furthermore, although our cost model (cf. §3.2) can represent any classification problem, in our evaluation we use CEF-SsL to assess binary classifiers. This is because the main goal of CTD is separating threats from legitimate events, but we acknowledge that more refined applications may involve fine-grained analyses. Evaluations of SsL methods in multi-classification settings are challenging, and we provide some considerations in Appendix D.

Labelling Accuracy. We assume that all the considered datasets are correctly labelled. However, such assumption may be overly optimistic: as described in §2, manual labelling is an error-prone task, and some recent papers highlighted that even well-known datasets may contain flaws (e.g., [151]). Due to the seminal nature of this SoK paper, we do not make any change to the provided labels—which also facilitates comparisons with previous works using such datasets, as the ground truth is the same. Nevertheless, we endorse future studies to question the correctness of the labelling procedures—especially if aimed at realistic deployments, as wrong labels induce data poisoning (which can also affect unlabelled samples [152]).

Concept Drift. Our evaluation assumes that the data distribution is stationary. In reality evaluations should be performed at regular intervals to prevent concept drift (cf. §3.2). Such operations, however, are facilitated by the design of our framework: CEF-SsL can also be applied to *lifelong learning* scenarios by selecting $\mathbb{F}$ and $\mathbb{L}$ on a temporal basis. For instance, in Tesseract [86], the initial model is developed under the assumption that all samples from the past are correctly labelled, resulting in over 50K samples. Our CEF-SsL can be applied by assuming that only a fraction of 'past' samples are correctly labelled ($\mathbb{L}$) while the remaining ones are not verified ($\mathbb{U}$), and the most recent samples are used as test ($\mathbb{F}$).

8. Conclusions

Acquiring ground truth information in CTD is difficult, but large amounts of unlabelled data are regularly available. These premises make SsL an intriguing opportunity, as it exploits unlabelled data to mitigate the problem of scarce ground truth. While many previous works have employed SsL for diverse CTD tasks, *none of them* investigated the benefit provided by unlabelled data. Despite being relatively cheap, such data still brings certain costs into the ML pipeline.

In this SoK paper, we specifically investigate the utility of unlabelled data and hence facilitate deployment of SsL methods for CTD. We formalize the evaluation requirements that enable one to assess the impact of unlabelled data in the development of a SsL model, under the assumption of a limited labelling budget. Prior works in this area had different scope and never considered such requirements, hence the impact of unlabelled data could not be assessed.

As a constructive demonstration, we provide an evaluation framework that meets all these requirements and use it to perform the first statistically validated benchmark of 9 selected SsL methods on 9 well-known datasets for CTD. The results reveal that only SsL methods using active learning are statistically better than baselines that do not use unlabelled data; however, in some cases they can degrade performance.

Our paper hence highlights the substantial margin for improvement of SsL methods for CTD. This motivates the quest for future contributions that exploit unlabelled data in CTD, compensating the high cost of expert knowledge in this field.

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Appendix A. Experimental Testbed

All our experiments are performed on a machine equipped with an Intel Xeon W-2195 CPU with 36 cores, 256GB RAM, 2TB SSD NVMe, and Nvidia Titan RTX GPU. The implementation leverages Python3 and the well-known ML library of scikit-learn. The specific ML algorithm used as base for all our models is the RandomForestClassifier. Training such classifier can be parallelized: in particular, we set the *njobs* parameter to use 34 cores (out of 36) of our CPU.

A.1. Data Preprocessing

NID datasets. The peculiarity of the considered NID datasets is that they all contain more than one malicious class.

- `CTU13` is composed of 13 PCAP traces, each one containing either benign or malicious traffic belonging to a given botnet family out of 7 possible families. Such traces are transformed into NetFlows via Argus. To prevent overfitting, we remove the full IP-address (we differentiate between internal/external IPs); we also derive some additional metrics (e.g., bytes per second, or the IANA port categories). The entire feature set is provided in Table 7, which is similar to the one in [153]. Then, we merge all sets according to the specific botnet family, obtaining 7 sets containing either benign samples, or malicious samples belonging to a single family. We exclude those botnet families with less than 1K samples.
- `IDS17` is provided as NetFlows, each separated in benign and malicious samples of different attacks. We use the entire feature set provided by the authors of `IDS17`, but we apply the same internal/external differentiation as done for `CTU13` to prevent overfitting on individual IP addresses. We aggregate the sets of NetFlows containing DoS attacks into a single set, and we exclude the families underrepresented. We create a dedicated set for the benign samples, which we use for all the experiments.
- `UNB15` the procedure is similar to `IDS17`. We use the same feature sets provided by the authors (with the usual distinction between internal/external machines). We aggregate the most represented families in 5 distinct sets.

TABLE 7: Features considered for `CTU13`.

#	Feature Name	Type
1	SrcIP internal	Bool
2	DstIP internal	Bool
3	SrcPort type	Cat
4	DstPort type	Cat
5	SrcPort	Cat
6	DstPort	Cat
7	Flow Duration $[s]$	Num
8	Flow Direction	Bool
9	Inc-Bytes	Num
10	Out-Bytes	Num
11	Total Bytes	Num
12	Incoming Packets	Num
13	Outgoing Packets	Num
14	Total Packets	Num
15	Bytes per Packet	Num
16	Bytes per Second	Num
17	Packets per Second	Num
18	Inc- per Out-Bytes	Num

The complete break down of the benign and malicious sets for each NID dataset is provided in Table 8.

TABLE 8: Breakdown of traces for NID datasets.

Dataset	Trace	Attack Class	Malicious Samples $\mathbb{D}_m$	Benign Samples $\mathbb{D}_b$
`CTU13`	1	Neris	246889	6473336
	2	e4f8	40904	2014041
	3	svchost	4630	554284
	4	qvodset	6127	2948062
	5	NSISay	2168	323300
	6	qvodset	143918	7104673
`UNB15`	1	DoS	16353	2218756
	2	Exploits	44525	
	3	Fuzzers	24246	
	4	Recon	13987	
`IDS17`	1	DoS	252661	2273097
	2	DDoS	128027	
	3	PortScan	158930	
	4	SshFtp	13835	
	5	WebAttack	2180	

In all experiments involving NID datasets, we devise ensemble of classifiers, each focused on a specific family (as done in [70], [153]). The results presented in our graphs are the average of all classifiers.

MD datasets. The task of MD has been tackled either as a binary classification [145] or as a multi-classification ML problem [9]—the latter focusing on identifying the specific malware family of a given sample. Because EMBER only has a single malicious family, all our MD are binary classifiers. To this purpose, we observe that DREBIN (collected from 2010 to 2012) has hundreds of malware families, some of which extremely underrepresented: hence, we considered the samples of top10 families and treated them as a single class. On the other hand, AndMal20 is more balanced across families, hence we consider all samples as a single malicious class.

PWD datasets. All PWD datasets include malicious samples of a single class. To the best of our knowledge, PWD has always been treated as a binary classification problem; hence, developing our PWD is more straightforward compared to NID and MD. The UCI and Mendeley datasets are provided directly as features; whereas for δPhish, we extract the most significant features based on the information of each provided webpage (HTML, URL, DNS) to achieve a similar feature set as the other two [53]. The queries to the DNS servers were performed in 2019, and some returned null results; we still consider these pages in our evaluation, as this happened for both benign and malicious pages. We provide in Table 9 the complete feature set used for δPhish.

TABLE 9: Features computed for the δPhish dataset.

URL-features	*REP-features*	*HTML-features*
IP address	SSL final state	SFH
'@' (at) symbol	URL/DNS mismatch	Anchors
'-' (dash) symbol	DNS Record	Favicon
Dots number	Domain Age	iFrame
Fake HTTPS	PageRank	MailForm
URL Length	PortStatus	Pop-Up
Redirect	Redirections	RightClick
Shortener		Objects
dataURI		StatusBar
		Meta-Scripts
		CSS

A.2. Developing the SsL models

We describe our SsL methods and provide an example.

'Pure' pseudo-labelling. We first use SL to predict the pseudo-labels of $\mathbb{U}$ and provide the confidence, c, of such predictions. Depending on c (see §6.2), the pseudo-labelled samples will be inserted in $\mathbb{L}$, resulting in a 'mixed' $\mathbb{L}$ used to train a 'pure' pseudo-labelling model. For the pseudo-labelling with retraining, we use πSsL to predict the labels of the remaining samples in $\mathbb{U}$, and assign those with $c \geq 99\%$ to $\mathbb{L}$ (with the pseudo-label).

'Pure' active learning. CEF-SsL composes another $\mathbb{L}$ (and another $\mathbb{U}$) with a two-step approach, by assuming that *half* of the labelling budget is used initially, and the remaining half is used for labelling the suggested samples. To this purpose, the initial $\mathbb{L}$ is changed by randomly removing half of its benign and malicious samples, therefore restoring the budget $\mathcal{L}$ to half of its initial value. Such $\mathbb{L}$ is used to train a 'support' SL model that predicts the labels of $\mathbb{U}$ and the corresponding confidence, c. CEF-SsL then simulates a human oracle that assigns the correct label to the samples that meet a confidence threshold (cf. §6.2) by accounting for such costs from the residual $\mathcal{L}$. Such samples, with their correct label, will be inserted in $\mathbb{L}$. To allow a fair comparison where all the models use an $\mathbb{L}$ with the same size, we assume that the cost for labelling each 'suggested' sample is standardized. This assumption is realistic, because it assumes that the sample already exists (it comes from $\mathbb{U}$) and a human operator can more efficiently verify a sample that is being provided with, compared to choosing and verifying samples randomly, or entirely creating new ones. The resulting new $\mathbb{L}$ (containing only correct labels) is then used to train the corresponding active learning model.

Pseudo-active models. We use the 'support' SL (trained on the 'halved' $\mathbb{L}$) to predict the pseudo labels of $\mathbb{U}$, and put all those with $c \geq 99\%$ in $\mathbb{L}$ (with the pseudo label). Such 'mixed' $\mathbb{L}$ is used to train a support πSsL, which predicts the remaining $\mathbb{U}$: the samples whose confidence meets the criteria in §6.2 are randomly put into the 'mixed' $\mathbb{L}$ until finishing the leftover budget. Such $\mathbb{L}$ (having the initial correct labels, the pseudo labels, and the 'suggested' correct labels) is used for training the pseudo-active SsL model.

Example. Consider the unbalanced case on CTU13 where $\mathcal{C}_m$=2$\mathcal{C}_b$, and $\mathcal{L}$=200 (cf. Table 3). For the 'pure' pseudo models and the baseline SL, the $\mathcal{L}$ is used all at the beginning, and the final $\mathbb{L}$ will always have 150 correctly labelled samples: 50 malicious samples and 100 benign. For active learning methods, the first half of the labelling budget (100) is used for the initial learner, by randomly choosing and removing 50 benign samples and 25 malicious samples from the previously randomly drawn $\mathbb{L}$; doing so leads to a smaller initial $\mathbb{L}$ with 75 samples. Then, because of our standardized assumption, the oracle will randomly assign the correct label to 75 samples that meet the desired confidence criteria, irrespective of their class. The oracle will *not* label more samples than what it is allowed by the budget. Nonetheless, the corresponding model will be tested on $\mathbb{F}$, and then the entire process is repeated 5 times to account for randomness in choosing the 'suggested' samples.

Appendix B. Benchmark

We present our benchmark evaluation, whose nature is *exploratory*: we are not interested in providing results that 'outperform' the state-of-the-art. Our focus is providing the first statistically validated benchmark for SsL methods in CTD and promote future analyses. Hence, we consider realistic scenarios where the amount of labelled data is scarce: in our evaluation, we never use more than 2.4K labelled samples. As a consequence, some results may appear to be underwhelming: we consider such outcomes to be *positive*, as they highlight the huge improvement margin concealed by SsL.

Results. The overall benchmark results are shown in Figs. 6 for NID datasets; Figs 7 for PWD datasets; and Figs 8 for MD datasets. Each figure consists in a set of 3 subfigures, each focused on a specific dataset. Every subfigure reports 3 plots, each focused on a specific 'balance' scenario (i.e., a specific $\mathcal{C}$). Every plot reports the F1-score (vertical axis) achieved by all the considered SsL methods (lines) for increasing labelling budgets $\mathcal{L}$ (horizontal axis). We observe that the performance of our MD for DREBIN (Fig. 8a) is significantly worse than on Ember (Fig. 8b) and on AndMal20 (Fig. 8c). Such phenomenon is due to our chosen aggregation strategy. Indeed, the considered malicious

samples in DREBIN belong to 10 different families; however, such samples are randomly chosen when composing the $\mathbb{L}$, i.e., $\mathbb{L}$ (which is very small) may not contain some families. As such, if these families are notably different from those included in $\mathbb{F}$ and—at the same time—vastly present in $\mathbb{F}$, then the MD will exhibit low performance. This phenomenon, however, does not appear in AndMal20 (for which we also aggregate families into a single class): an explanation is that the malicious families in AndMal20 are more similar to each other than those included in DREBIN.

How many experiments does the benchmark include? We report in Table 10 the overall number of models considered in our evaluation. Specifically, for each dataset we report n, k and the corresponding N. Multiplying all of these numbers yields the 'runs' of any model that does not leverage active learning, i.e., $\overline{SL}$, SL, $\underline{SsL}$, $\pi\,SsL$, $\widehat{\pi}\,SsL$. Because we draw the samples for active learning randomly and we repeat such draw 5 times for each corresponding model, all the 6 active learning models (i.e., $\alpha\,SsL_h$, $\alpha\,SsL_o$, $\alpha\,SsL_l$, $\alpha^{\pi}\,SsL_h$, $\alpha^{\pi}\,SsL_o$, $\alpha^{\pi}\,SsL_l$) are assessed 5 times as much. Hence, for every line in a given plot, each 'point' is the average results of as many models as reported in Table 10. As an example, on CTU13, each point in a given plot of Fig. 6a is the average F1-score of 990 models if the line is related to an active learning method, or 198 models if not—all of which evaluated for the corresponding value of $\mathcal{L}$ and cost scenario $\mathcal{C}$.

TABLE 10: Total amount of results considered for each 'point' in Figs 6–8.

CTD (Figure)	Dataset (Subfigure)	n, k	N	Active models (6)	Other models (5)
NID Figs. 6	CTU13 (Fig. 6a)	(11,3)	6	990	198
	UNB15 (Fig. 6b)	(23,4)	4	1840	368
	IDS17 (Fig. 6c)	(15,3)	5	1125	225
PWD Figs. 7	UCI (Fig. 7a)	(20,5)	1	500	100
	Mendeley (Fig. 7b)	(20,5)	1	500	100
	δPhish (Fig. 7c)	(20,5)	1	500	100
MD Figs. 8	Drebin (Fig. 8a)	(20,5)	1	500	100
	Ember (Fig. 8b)	(20,5)	1	500	100
	AndMal20 (Fig. 8c)	(20,5)	1	500	100

All the values in Table 10 correspond *only* to a specific combination of $\mathcal{L}$ and $\mathcal{C}$, meaning that the overall amount of models developed in our evaluation is 12 times as much—for each dataset. In summary, the results of SoK paper correspond to 500 760 active learning models and 83 460 non-active learning models, for a total of 584 220 models.

Appendix C. Case Study: Comparison with a prior work

Let us discuss a case study where we compare our evaluation with a recent work sharing a similar testbed.

The combination of pseudo labelling and active learning has been investigated also by Zhang et al. [70] on CTU13 and IDS17 by using–among others–the same confidence levels as our implementation: above 99% for the pseudo labelling, and below 1% for active learning (making it equivalent to our $\pi\,SsL$ and $\alpha\,SsL_l$). In [70], the two source datasets (IDS17 and CTU13) are divided into a single set of benign samples; whereas the malicious samples are distributed into several sets depending on their attack family, and then aggregated into a single malicious class. This is a valid operation, but it slightly differs from our testbed, because we treat malicious classes separately for each NID dataset.

Let us describe the evaluation methodology of [70]. Our first observation is that, after 'preprocessing' the source datasets, the authors of [70] obtain 100K samples for CTU13 and 600K samples for IDS17. In contrast, after preprocessing, we obtain 20M samples for CTU13 and 3M for IDS17—and this is despite removing some underrepresented families (cf. Table 2). We are not aware of the reason of this gap, but also other studies (e.g., [153], [154]) obtain similar compositions as ours.

Regardless, each preprocessed dataset in [70] is further filtered to obtain $\mathbb{D}$, which contains 15K benign samples and 9K malicious samples. Such $\mathbb{D}$ (which represents only a small portion of all their preprocessed traffic, i.e. 10% for CTU13, and 4% for IDS17) is *never* changed during their experiments, and the remaining samples are *never* used. In contrast, we consider as $\mathbb{D}$ the entire datasets after preprocessing.

Then, the authors of [70] partition such $\mathbb{D}$ into $\overline{\mathbb{L}}$ and $\mathbb{F}$ by using a 70:30 split (we use 80:20), resulting in a $\overline{\mathbb{L}}$ with 17K samples, and a $\mathbb{F}$ with 7K samples—both having ρ=(62,38). The split is done randomly, but the process is never repeated and the $\mathbb{F}$ stays the same for the entire evaluation. What would have happened if $\mathbb{F}$ contained different samples? We address this issue by changing $\mathbb{F}$ multiple times (k) for each malicious class (N), meaning 18 times for CTU13, and 15 times for IDS17.

To obtain their $\mathbb{L}$ (and corresponding $\mathbb{U}$), the authors of [70] isolate a variable portion of samples from $\overline{\mathbb{L}}$, specifically either 5%, 10% or 20% (hence, the correct labels in their $\mathbb{L}$ range from ∼1K to ∼4K). The choice of samples put in $\mathbb{L}$ is done randomly in [70], but the experiments are repeated only 10 times. In contrast, we do so n times for each new $\mathbb{F}$, meaning that we do so 198 times for CTU13 and 225 times for IDS17. This increases the confidence of our results. Moreover, we also consider different balance ratios, whereas the balancing in [70] is always a fixed ρ=(62,38) for all sets.

Finally, in [70] they consider the SL baseline, but neglect the $\underline{SsL}$ baseline and the $\overline{SL}$ baseline. Both lacks are significant: without $\underline{SsL}$, it is not possible to estimate the least possible benefit provided by $\mathbb{U}$ (if any); without $\overline{SL}$, it is not possible to determine any upper bound in performance. If the SL is not far from $\overline{SL}$, then it may not be worth in investing in $\mathcal{U}$ for using SsL methods.

Let us compare our results, with the aim of pinpointing what 'issues' prevent deriving actionable conclusions on the impact of unlabelled data in [70]. For simplicity, we focus on the F1-score achieved on CTU13 (cf. Fig.6a). The baseline SL in [70] achieves a lower performance than ours despite being trained on more samples: the one in [70] obtains 0.81 F1-score when trained on 4000 samples, whereas our baseline SL trained with an $\mathbb{L}$ of 2400 samples (the highest we considered) reached 0.87 F1-score, as evidenced by the rightmost plot in Fig.6a. When applying pseudo-labelling in [70], the performance increases from 0.81 to 0.83 F1-score. All these results contrast with ours, because the performance of our corresponding model, $\pi\,SsL$, is lower than the baseline. However, while our results take into account a total of 198 trials, the ones in [70] are performed only 10 times,

which is hardly enough to make any informed decision on whether it is truly convenient to invest in $\mathcal{U}$.

Finally, the authors of [70] do not maintain the original $\mathcal{L}$ when applying active learning, and do not report how many samples require to be 'actively labelled' as they inject all those within the confidence threshold (below 1%) into $\mathbb{L}$ (as also done in Tesseract [86]), making any comparison with our models (and, also, with their baselines) unfair.

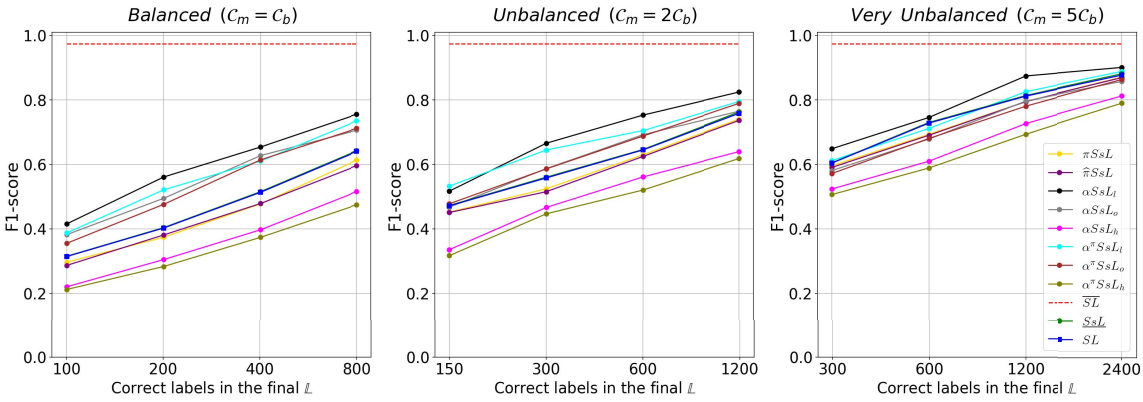
We can conclude that the evaluation performed in [70] can only show that, under certain conditions, some SsL methods can improve the performance. However, the results obtained cannot certify that such improvement is significant, because they are conducted in a fixed setting (same $\mathbb{F}$, same balance ratio, only 10 runs), despite being performed on two datasets. Hence, the question "do I need $\mathbb{U}$?" is still open.

Appendix D. CEF-SsL for multi-classification

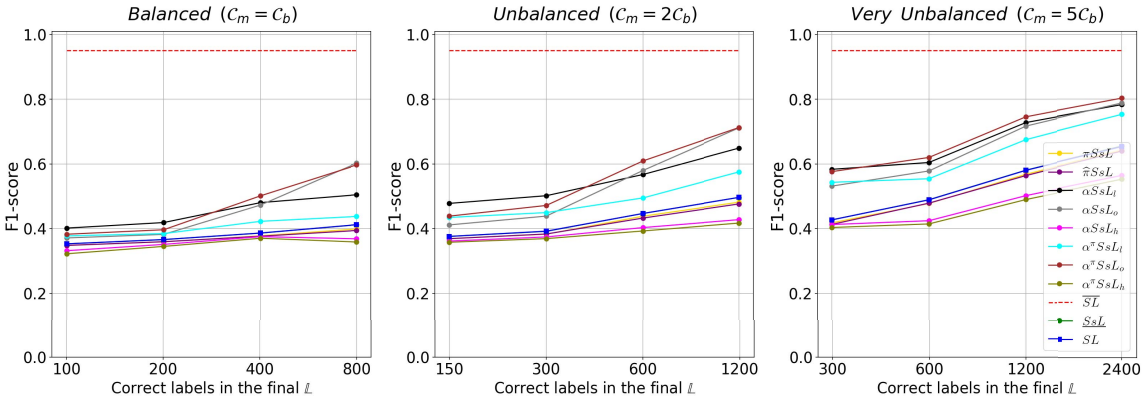
In our evaluation we treat CTD as a binary classification problem, where a sample is either benign or malicious. The motivation is that N+1 classification (with N>1) assumes a 'closed world' scenario where all malicious classes are known beforehand, which is hardly the case in the dynamic cybersecurity landscape. Nevertheless, some specific applications may favor SsL method devoted to multi-classification: applying CEF-SsL in similar settings is possible, i.e., by manually specifying the cost to label *each* malicious sample $\mathcal{C}_x$, and performing hundreds of runs of CEF-SsL—but this is empirically difficult from a research perspective. Some alternatives exist, but they are also challenging.

The main challenge is *randomly choosing a limited amount of samples from N malicious classes*. For instance, some datasets (e.g., DREBIN) only have a very limited number of samples for some classes; a possible workaround is applying some aggregation techniques and create some 'macro' classes; however, such approach may introduce some experimental bias. Another option is removing those classes for which only few samples are available: in this case, however, the ML model may perform poorly if such families 'appear' after the model is deployed. To mitigate such problem, all underrepresented classes can be merged into a dedicated 'other' class: the ML model may retain some performance at inference; but it may also be confused when the more represented classes present similarities with the samples of the 'other' class.

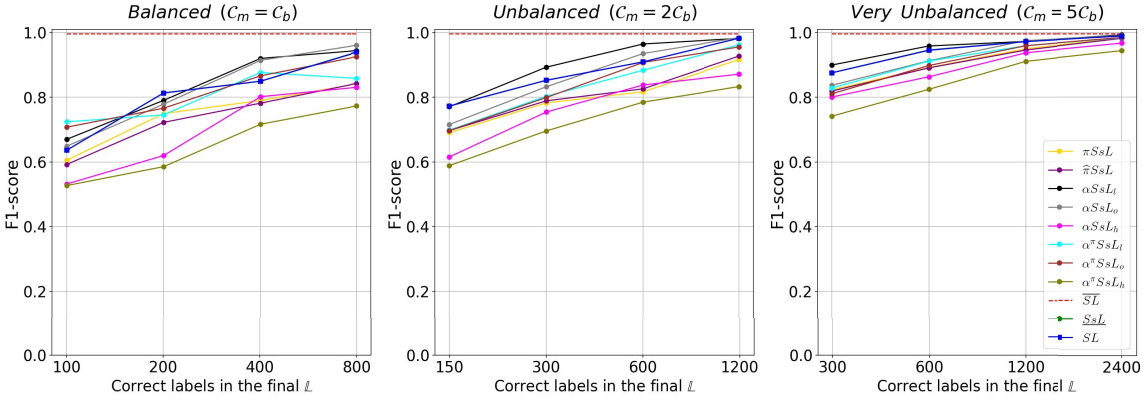
Another challenge is *composing 'appropriate'* partitions, i.e., $\mathbb{L}$, $\mathbb{U}$ and $\mathbb{F}$. It is well-known that, in reality, benign events are more abundant than malicious ones, and it is common to compose train/test partitions where benign samples are the majority. However, when malicious samples belong to different classes and the labeling budget is limited, it begs the question of "how many samples *per class* should be included in $\mathbb{L}$?". As an example, assume that $\mathcal{L}$=500; how should $\mathbb{L}$ be composed when a dataset contains 10K benign samples, alongside three malicious classes, the first with 2000 samples, the second with 100 samples, and the third with 50 samples? And what about $\mathbb{U}$ and $\mathbb{F}$? A possibility is using the relative distribution in a given dataset, but it may induce bias or skew the model into favoring the majority class. Conversely, it is possible to infer which family is more popular 'in the wild', but this may require extra resources to study updated security feeds.



(a) Results on **CTU13**. For every plot, each 'point' represents the average results of 198 models (and 5 times as many for all models using active learning).

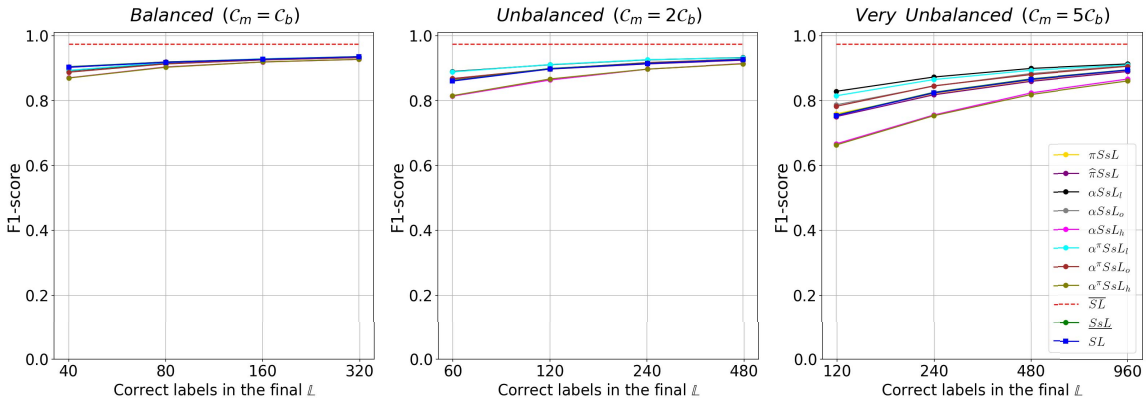


(b) Results on **UNB15**. For every plot, each 'point' represents the average results of 368 models (and 5 times as much for all models using active learning).

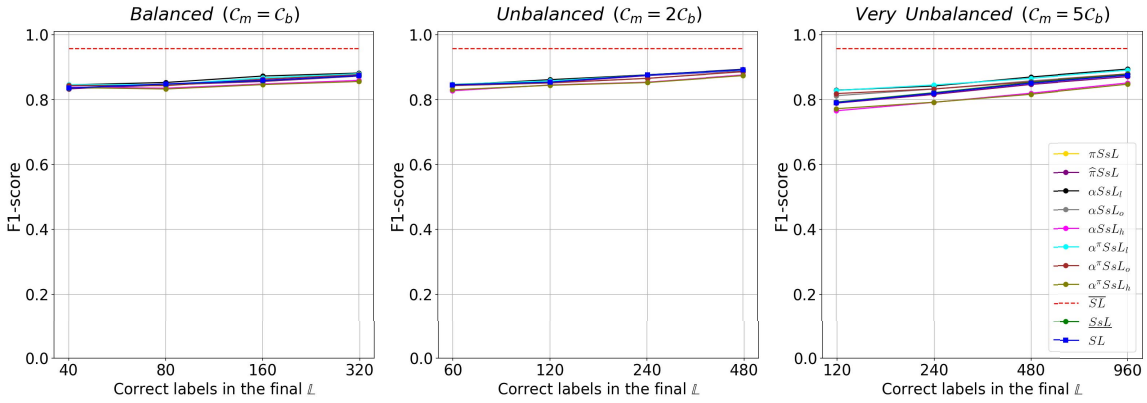


(c) Results on **IDS17**. For every plot, each 'point' represents the average results of 225 models (and 5 times as much for all models using active learning).

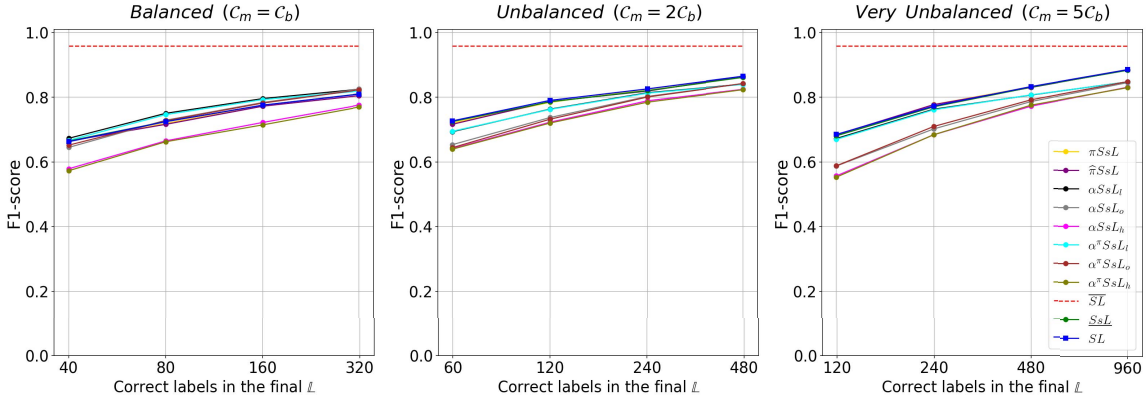
Figure 6: **Network Intrusion Detection**. For each dataset, we report the results for the three cost (or balancing) scenarios. Each scenario is shown in a plot, where the y-axis reports the F1-score and the x-axis the (increasing) labelling budget. Each method is denoted with a line on each plot.



(a) Results on **UCI**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).

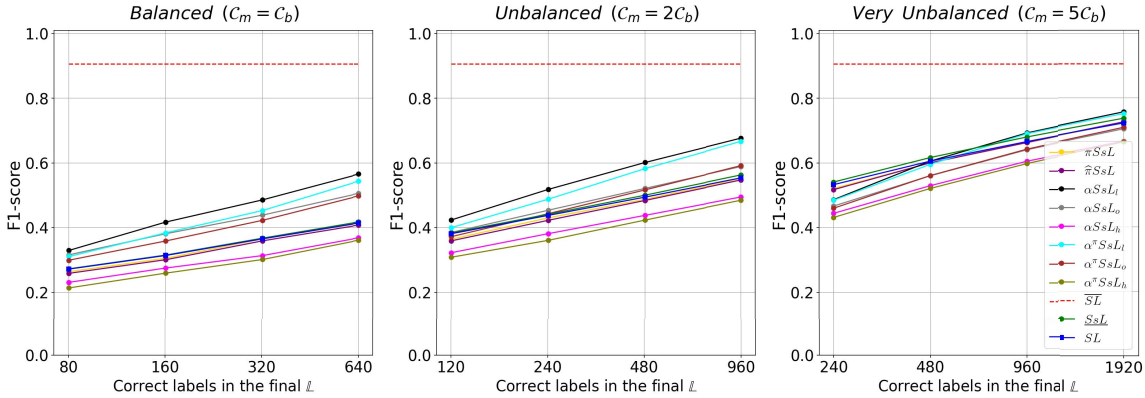


(b) Results on **Mendeley**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).

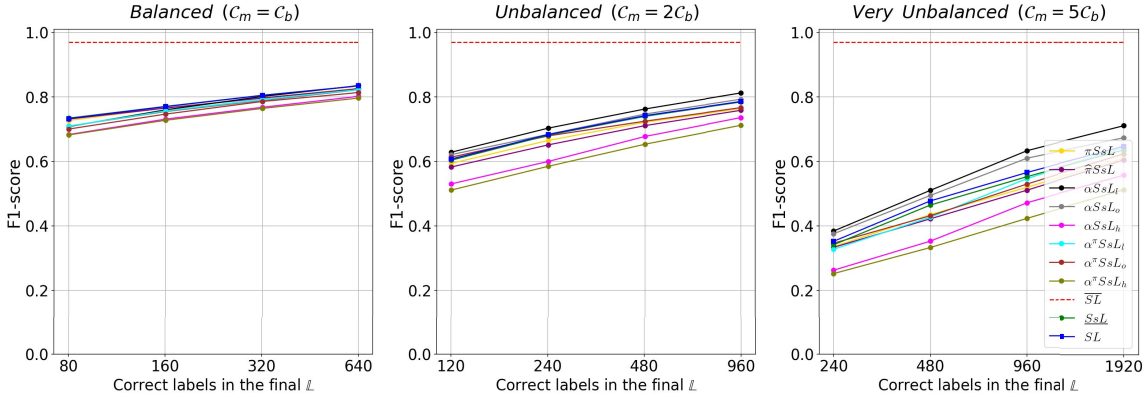


(c) Results on δ**Phish**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).

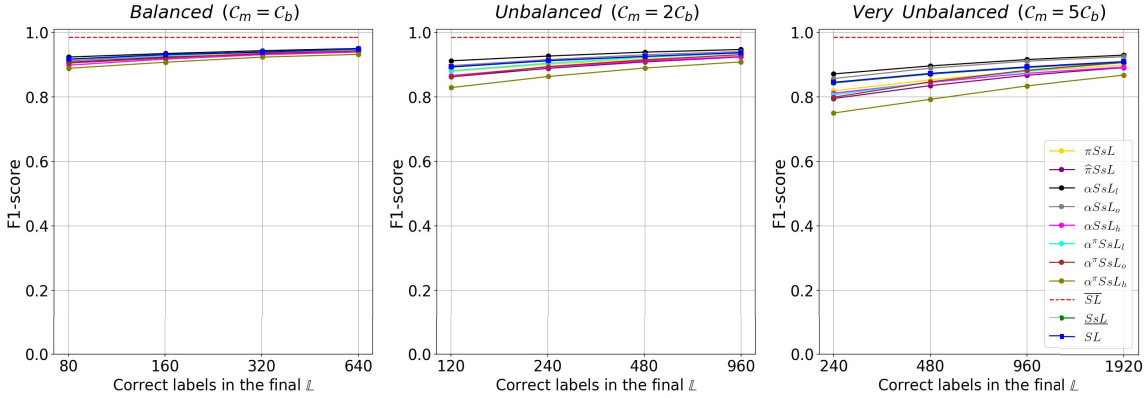
Figure 7: **Phishing Website Detection**. For each dataset, we report the results for the three cost (or balancing) scenarios. Each scenario is shown in a plot, where the y-axis reports the F1-score and the x-axis the (increasing) labelling budget. Each method is denoted with a line on each plot.



(a) Results on **DREBIN**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).



(b) Results on **Ember**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).



(c) Results on **AndMal20**. For every plot, each 'point' represents the average results of 100 models (and 5 times as much for all models using active learning).

Figure 8: **Malware Detection**. For each dataset, we report the results for the three cost (or balancing) scenarios. Each scenario is shown in a plot, where the y-axis reports the F1-score and the x-axis the (increasing) labelling budget. Each method is denoted with a line on each plot.